



US Army Corps
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Waterways Experiment
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Technical Report CHL-98-19
July 1998

A Numerical Model Simulating Water Flow and Contaminant and Sediment Transport in WaterShed Systems of 1-D Stream-River Network, 2-D Overland Regime, and 3-D Subsurface Media (WASH123D: Version 1.0)

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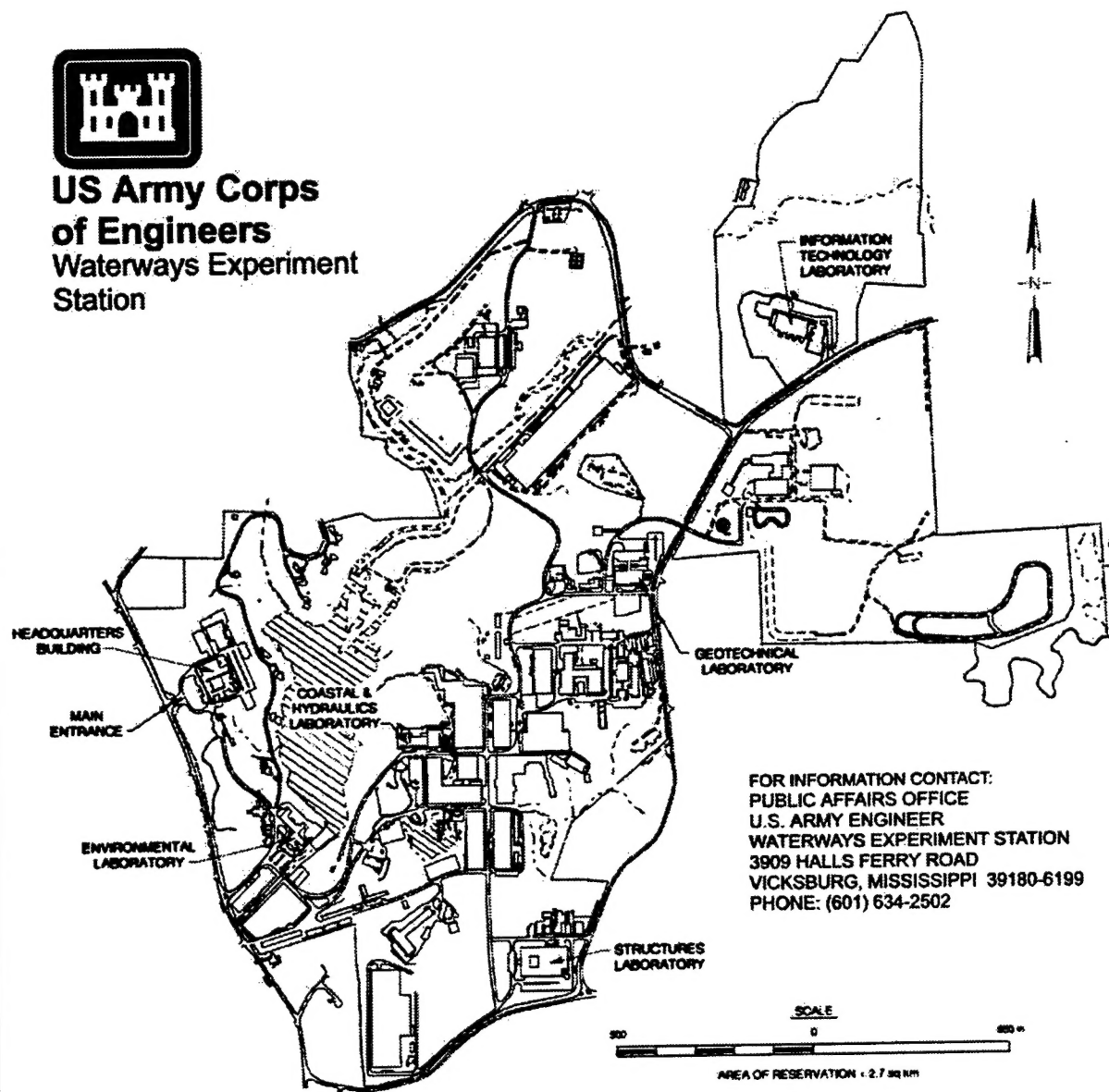
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Waterways Experiment Station Cataloging-in-Publication Data

A numerical model simulating water flow and contaminant and sediment transport in WaterSHed systems of 1-D stream-river network, 2-D overland regime, and 3-D subsurface media (WASH123D: version 1.0) / by Gour-Tsyh (George) Yeh ... [et al.] ; prepared for U.S. Environmental Protection Agency, Environmental Research Laboratory.

369 p. : ill. ; 28 cm. -- (Technical report ; CHL-98-19)

Includes bibliographic references.

1. Groundwater -- Pollution -- Mathematical models. 2. Sediment transport -- Mathematical models. 3. WASH123D (Computer program) 4. Watersheds -- Mathematical models. I. Yeh, Gour-Tsyh. II. United States. Army. Corps of Engineers. III. U.S. Army Engineer Waterways Experiment Station. IV. Coastal and Hydraulics Laboratory (U.S. Army Engineer Waterways Experiment Station) V. Title: WASH123D VI. United States. Environmental Protection Agency. VII. Environmental Research Laboratory (Athens, Ga.) VIII. Series: Technical report (U.S. Army Engineer Waterways Experiment Station) ; CHL-98-19.
TA7 W34 no.CHL-98-19

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Figure I.1 Specification of 3-D element sides.

Preface

This study was conducted for the U.S. Environmental Protection Agency (EPA) Environmental Research Laboratory, Athens, GA. Dr. Bob Carsel, EPA Athens Environmental Research Laboratory, was point of contact for the study.

The study was conducted in the Hydraulics Laboratory (HL) of the U.S. Army Engineer Waterways Experiment Station (WES) from 1995 to 1997 under the direction of Mr. Frank. A. Herrmann, Jr., Director, HL; Mr. Richard. A. Sager, Assistant Director, HL; and Dr. William D. Martin, Chief, Hydro-science Division, (HD), HL.

The report was prepared by Drs. Gour-Tsyh (George) Yeh, Hwai-Ping (Pearce) Cheng, and Jing-Ru (Ruth) Cheng, Pennsylvania State University, University Park, PA; and Drs. Hsin-Chi J. Lin and William D. Martin, Watershed Systems Group, Estuaries and Hydro-science Division.

This report is being published by the WES Coastal and Hydraulics Laboratory (CHL). The CHL was formed in October 1996 with the merger of the WES Coastal Engineering Research Center and Hydraulics Laboratory. Dr. James R. Houston is the Director of the CHL and Mr. Charles C. Calhoun, Jr., is the Assistant Director.

At the time of publication of this report, Director of WES was Dr. Robert W. Whalin. Commander was COL Robin R. Cababa, EN.

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Section 1. INTRODUCTION

This report is to present a numerical model designed to simulate water flow and chemical and sediment transport in watershed systems. This watershed model includes a 1-D river/stream network flow module, a 1-D river/stream network transport module, a 2-D overland flow module, a 2-D overland transport module, a 3-D subsurface flow module, and a 3-D subsurface transport module to link surface and subsurface systems through infiltration/seepage. This watershed model can be used to simulate flows alone, sediment transport alone, reactive chemical transport alone, or flow and sediment and reactive chemical transport simultaneously. This model can read flow fields computed from either its flow module or other flow models to proceed transport simulations. When both flow and transport are simulated, the flow fields are computed first. Then the transport is calculated using the computed flow fields at respective times. The feedback of transport on flow is not considered (e.g., no density effect is considered) in this model.

There may be three approaches to model surface flow in a watershed system: the kinematic, diffusive, and dynamic wave models. The dynamic wave models completely describe water flow but they are very difficult to solve under some conditions (e.g., when the slope of ground surface is steep), regardless of what numerical approach is employed. On the other hand, the diffusion and/or kinematic models can handle a wide range of flow problems but are inaccurate when the inertial terms play significant roles (e.g., when the slope of groundwater surface is small). Thus, three options are provided in this report: the kinematic wave model, the diffusion wave model, and the dynamic wave model to accurately compute water flow over a wide range of conditions. The diffusion/kinematic wave models were numerically approximated with the Lagrangian method. The dynamic model was first mathematically transformed into characteristic wave equations. Then it was numerically solved with the Lagrangian-Eulerian method.

The subsurface flow governing equations are discretized with the Galerkin finite element method. The surface/subsurface interface boundary is treated as a variable boundary as described in the FEMWATER mode (Yeh, 1987).

The principles of mass balance were employed to derive the transport equations governing the temporal-spatial distribution of chemicals, suspended sediment, and bed sediment. Chemical kinetics based on the collision theory was used to present the relationship between reactant and product species in all chemical reactions and volatilization. The predictor-corrector numerical scheme was used to solve the transport equations. In the predictor step, the Lagrangian-Eulerian method was employed to solve the advection-dispersion transport equation with the source/sink term evaluated at the previous time. In the corrector step, the implicit finite difference was used to solve the system of ordinary equations governing the chemical kinetic reactions. The nonlinearity in flow and sediment transport equations is handled with the Picard method, while the nonlinear chemical system is solved by using the Newton-Raphson method.

In the following, Section 2 provides a heuristic derivation of the governing equations for flow in river/stream network (Section 2.1), surface runoff in the overland regime (Section 2.2), flow in the subsurface (Section 2.3) sediment and chemical transport in river/stream network (Section 2.4), sediment and chemical transport in the overland regime (Section 2.5), and chemical transport in the subsurface (Section 2.6). Section 3 includes numerical approaches to solve governing equations for flows in the river/stream network, overland, and subsurface systems. Dynamic wave and kinematic/diffusion wave models are both given for solving flow on ground surface. This section also describes the numerical approximation to solve both sediment and chemical transport in river/stream network and overland regimes, and chemical transport in the subsurface as well. Section 4 gives 15 groups of example problems to illustrate

the capability of the model. These include: (1) 1-D flow, (2) 2-D flow, (3) 1-D transport, (4) 2-D transport, (5) 1-D flow and transport, (6) 2-D flow and transport, (7) 1-D/2-D flow, (8) 1-D/2-D flow and transport, (9) 3-D flow, (10) 3-D transport, (11) 3D flow and transport, (12) 2-D/3D flow, (13) 2-D/3-D flow and transport, (14) 1-D/2-D/3-D flow, and (15) 1-D/2-D/3-D flow and transport. A summary and continuing work are given in Section 5. A data input guide is presented in Appendix I, program structure and subroutine are described in Appendix II, and required parameters to run the model are listed in Appendix III.

Section 2. MATHEMATICAL BASIS

In this section, we present give governing equations, initial conditions, and boundary conditions for simulating water flow and chemical and sediment transport in watershed systems.

2.1. Water flow in 1-D river/stream

The governing equations of water flow in 1-D river/stream can be derived based on the conservation law of water mass and linear momentum [Singh, 1996], and can be written as follows.

The continuity equation:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = S_s + S_R - S_I + S_1 + S_2 \quad (2.1)$$

where t is time [T]; x is the axis along the river/stream direction [L]; A is cross-sectional area of the river/stream [L^2]; Q is flow rate of the river/stream [L^3/T]; S_s is the man-induced source [L^2/T]; S_R is the source due to rainfall [L^2/T]; S_I is the sink due to infiltration [L^2/T]; S_1 and S_2 are the source terms contributed from overland flow [L^2/T].

The momentum equation:

$$\frac{\partial Q}{\partial t} + \frac{\partial uQ}{\partial x} = -gA \frac{\partial(Z_0 + h)}{\partial x} + \frac{\partial F_x}{\partial x} + u^r S_R - u^i S_I + u^{Y1} S_1 + u^{Y2} S_2 + \frac{T^s - T^b}{\rho} \quad (2.2)$$

where h is water depth [L]; u is river/stream velocity [L/T]; g is gravity [L/T^2]; Z_0 is bottom elevation [L]; F_x is the momentum flux due to eddy viscosity [L^4/T^2]; u^r is the velocity of rainfall along the river/stream direction [L/T]; u^i is the velocity of infiltration along the river/stream direction [L/T]; u^{Y1} and u^{Y2} are the velocity, along the river/stream direction [L/T], of water from overland to river/stream; ρ is water density [M/L^3]; T^s is surface shear stress [M/T^2]; T^b is bottom shear stress [M/T^2].

Eqs. (2.1) and (2.2) are the governing equations of a 1-D dynamic wave river/stream flow model. When the diffusion wave model is considered, however, the inertia terms along the momentum equation is assumed negligible when compared with the other terms. By further assuming negligible surface shear stress, negligible eddy viscosity, and $u^r = u^i = u^{Y1} = u^{Y2} = 0$, we approximate the river/stream velocity with the following equation (Hergarten and Neugebauer, 1995).

$$u = \frac{-1}{n} \left[\frac{R}{1 + (\nabla Z_0)^2} \right]^{2/3} \frac{1}{(\nabla(Z_0 + h))^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \quad (2.3)$$

where n is Manning's roughness; R is hydraulic radius [L], which is defined as $R(x,t) = R^*(x,h(x,t)) = A/P$, P is the wetted perimeter [L] and can be expressed as $P(x,t) = P^*(x,h(x,t))$.

To achieve transient simulations, either water depth or stage must be given as the initial condition, as well as flow velocity. In addition, appropriate boundary conditions need to be specified to match the corresponding physical system. In the model, four types of boundary conditions are taken into account and are stated as follows.

Water depth- or stage-specified boundary condition:

This condition is applied when either water depth or stage can be prescribed at the river/stream boundary through the simulation time of period. Such a condition can be expressed as

$$h(x_b, t) = h_b(t) \quad (2.4)$$

or

$$h(x_b, t) + Z_0(x_b) = H_b(t) \quad (2.5)$$

where x_b is the coordinate of a river/stream boundary; $h_b(t)$ is a prescribed time-dependent water depth [L]; $H_b(t)$ is a prescribed time-dependent water stage [L].

Flow rate-specified boundary condition:

This condition is employed when the time-dependent incoming flow rate can be prescribed at a upstream river/stream boundary. It can be expressed as

$$Q(x_b, t) = u(x_b, t)A(x_b, t) = Q_b(t) \quad (2.6)$$

where $Q_b(t)$ is a time-dependent flow rate [L^3/T].

Water depth-dependent flow rate boundary condition:

This condition is often used to describe the flow rate at a downstream river/stream boundary at which the flow rate is a function of water depth. It can be written as

$$Q(x_b, t) = u(x_b, t)A(x_b, t) = Q_b(h(x_b, t)) \quad (2.7)$$

where $Q_b(h(x_b, t))$ is a water depth-dependent flow rate [L^3/T].

Junction boundary condition:

This condition is applied to a boundary of a river/stream reach when the boundary is connected to a junction. In this case, the stage of the boundary is specified as the stage of the junction. That is,

$$h(x_b, t) + Z_0(x_b) = H_{\text{junction}}(t) \quad (2.8)$$

$H_{\text{junction}}(t)$ is the water stage [L] at the junction that is computed through the computation of water budget. We will give the detail of computing $H_{\text{junction}}(t)$ in Section 3.

2.2. Water flow in 2-D overland

The governing equations of 2-D overland flow can be derived based on the conservation law of water mass and linear momentum [Wang and Connor, 1975]. The governing equations of a dynamic wave model can be written as follows.

The continuity equation:

$$\frac{\partial h}{\partial t} + \frac{\partial uh}{\partial x} + \frac{\partial vh}{\partial y} = SS + R - I \quad (2.9)$$

where h is water depth [L]; u is the x-velocity [L/T]; v is the y-velocity [L/T]; SS is the man-induced source [L/T]; R is the source due to rainfall [L/T]; I is the sink due to infiltration [L/T].

The x-momentum equation:

$$\frac{\partial uh}{\partial t} + \frac{\partial u^2 h}{\partial x} + \frac{\partial uvh}{\partial y} = -gh \frac{\partial(Z_0 + h)}{\partial x} + \frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y} + (u^r R - u^i I) + \frac{\tau_x^s - \tau_x^b}{\rho} \quad (2.10)$$

where Z_0 is the bottom elevation of overland [L]; u^r is the component of rainfall velocity along the x-direction [L/T]; u^i is the component of infiltration velocity along the x-direction [L/T]; F_{xx} and F_{yx} are the fluxes due to eddy viscosity along the x-direction [L³/T²]; τ_x^s is the component of surface shear stress along the x-direction over unit horizontal overland area [M/L/T²]; τ_x^b is the component of bottom shear stress along the x-direction over unit horizontal overland area [M/L/T²].

The y-momentum equation:

$$\frac{\partial vh}{\partial t} + \frac{\partial uvh}{\partial x} + \frac{\partial v^2 h}{\partial y} = -gh \frac{\partial(Z_0 + h)}{\partial y} + \frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y} + (v^r R - v^i I) + \frac{\tau_y^s - \tau_y^b}{\rho} \quad (2.11)$$

where v^r is the component of rainfall velocity along the y-direction [L/T]; v^i is the component of infiltration velocity along the y-direction [L/T]; F_{xy} and F_{yy} are the fluxes due to eddy viscosity along the y-direction [L³/T²]; τ_y^s is the component of surface shear stress along the y-direction over unit horizontal overland area [M/L/T²]; τ_y^b is the component of bottom shear stress along the y-direction over unit horizontal overland area [M/L/T²].

In Eqs. (2.10) and (2.11), it is noted that if $R > 0$, u^r and v^r are prescribed; otherwise, $u^r = u$ and $v^r = v$. Likewise, if $I < 0$, u^i and v^i are either prescribed or computed with subsurface flow models; otherwise, $u^i = u$ and $v^i = v$.

When the diffusion wave model is considered, the inertia terms in Eqs. (2.10) and (2.11) are assumed not important when compared to the others. With the further assumption that eddy viscosity is insignificant, surface shear stress is negligible, and $u^r = v^r = u^i = v^i = 0$, we approximate the velocity (u , v) as follows.

$$u = \frac{-1}{n} \left[\frac{h}{1 + (\nabla Z_0)^2} \right]^{2/3} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \quad (2.12)$$

$$v = \frac{-1}{n} \left[\frac{h}{1 + (\nabla Z_0)^2} \right]^{2/3} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial y} \quad (2.13)$$

To perform transient simulations, water depth (or stage) and velocity must be given as the initial conditions. Four types of boundary conditions are implemented in the model, as described as follows.

Water depth- or stage-specified boundary condition:

This condition is applied when either water depth or stage can be prescribed at overland boundary nodes through the simulation time of period. Such a condition can be expressed as

$$h(x_b, y_b, t) = h_b(t) \quad (2.14)$$

or

$$h(x_b, y_b, t) + Z_0(x_b, y_b) = H_b(t) \quad (2.15)$$

where (x_b, y_b) is the coordinate of a overland boundary node; $h_b(t)$ is a prescribed time-dependent water depth [L]; $H_b(t)$ is a prescribed time-dependent water stage [L].

Normal flux-specified boundary condition:

This condition is employed when the time-dependent incoming normal flux can be prescribed at a upstream overland boundary segment. It can be expressed as

$$-\mathbf{n} \cdot \mathbf{q}(x_b, y_b, t) = -\mathbf{n} \cdot \mathbf{V}(x_b, y_b, t) h(x_b, y_b, t) = q_b(t) \quad (2.16)$$

where \mathbf{n} is the outward unit normal vector of the boundary segment; $\mathbf{V} = (u, v)$; $q_b(t)$ is a time-dependent normal flux [L^2/T].

Water depth-dependent normal flux boundary condition:

This condition is often used to describe the outgoing normal flux at a downstream overland boundary segment at which the flux is a function of water depth. It can be written as

$$-\mathbf{n} \cdot \mathbf{q}(x_b, y_b, t) = -\mathbf{n} \cdot \mathbf{V}(x_b, y_b, t) h(x_b, y_b, t) = -q_b(h(x_b, y_b, t)) \quad (2.17)$$

where $q_b(h(x_b, y_b, t))$ is a water depth-dependent normal flux [L^2/T].

River/stream- or junction-related boundary condition:

This condition is applied to a overland boundary segment when the boundary segment is next to a river/stream or a junction, and through the segment water may flow from overland to river/stream or from river/stream to overland, depending on the water stages at both river/stream and overland. In this occasion, the normal flux is computed based on either the water depth on the overland boundary or the difference between overland and river/stream water stages. Three cases are included in this type of boundary condition.

< Case 1 > River/stream water stage is lower than the bottom elevation of the overland boundary.

In this case, water is injected to river/stream from overland. The normal flux can be expressed as

$$-\mathbf{n} \cdot \mathbf{q}(x_b, y_b, t) = -\mathbf{n} \cdot \mathbf{V}(x_b, y_b, t) h(x_b, y_b, t) = -q_b(h(x_b, y_b, t)) \quad (2.18)$$

where $q_b(h(x_b, y_b, t))$ is a water depth-dependent normal flux [L^2/T].

< Case 2 > River/stream water stage is higher than the bottom elevation of the overland boundary but is lower than the water stage of the overland boundary.

In this case, water is still injected to river/stream from overland. The normal flux can be expressed as

$$-\mathbf{n} \cdot \mathbf{q}(x_b, y_b, t) = -\mathbf{n} \cdot \mathbf{V}(x_b, y_b, t) h(x_b, y_b, t) = -q_b(\Delta H(x_b, y_b, t)) \quad (2.19)$$

$$\Delta H(x_b, y_b, t) = H(x_b, y_b, t) - H_c(x_c, t) \quad (2.20)$$

where $H(x_b, y_b, t)$ is the water stage on the overland boundary [L]; $H_c(x_c, t)$ is the water stage at the river/stream related to the overland boundary [L]; ΔH is the stage difference between river/stream and overland [L]; $q_b(\Delta H(x_b, y_b, t))$ is a stage difference-dependent normal flux [L^2/T].

< Case 3 > River/stream water stage is higher than the water stage of the overland boundary.

In this case, water flows from river/stream to overland. The normal flux can be expressed as

$$-\mathbf{n} \cdot \mathbf{q}(x_b, y_b, t) = -\mathbf{n} \cdot \mathbf{V}(x_b, y_b, t) h(x_b, y_b, t) = q_b(\Delta H(x_b, y_b, t)) \quad (2.21)$$

$$\Delta H(x_b, y_b, t) = H_c(x_c, t) - H(x_b, y_b, t) \quad (2.22)$$

where $q_b(\Delta H(x_b, y_b, t))$ is a stage difference-dependent normal flux [L^2/T].

2.3. Water flow in 3-D subsurface

The governing equation of subsurface flow through saturated-unsaturated porous media can be derived based on the conservation law of water mass [Yeh, 1987]. It is written as follows.

$$\frac{\partial \theta}{\partial t} + \nabla \cdot \mathbf{V} = F \frac{\partial h}{\partial t} + \nabla \cdot [-\mathbf{K} \cdot (\nabla h + \nabla z)] = q \quad (2.23)$$

where h is the pressure head [L]; t is time [T]; \mathbf{K} is the hydraulic conductivity tensor [L/T]; z is the potential head [L]; q is the source and/or sink [L^3/L^3]; and F is the water capacity [$L^3/L^3/T$] given by

$$F = \frac{d\theta}{dh} \quad (2.24)$$

in which θ is the moisture content [L^3/L^3].

To achieve transient simulation, the following initial condition needs to be given.

$$h = h_i(x, y, z) \quad \text{in } R, \quad (2.25)$$

where R is the region of interest and h_i is the prescribed pressure head [L], which can be obtained by either field measurements or by solving the steady state version of Eq. (2.23).

Five types of boundary conditions are taken into account as follows.

Dirichlet conditions:

This boundary condition is used when pressure head can be prescribed on the boundary. It can be expressed as

$$h = h_d(x_b, y_b, z_b, t) \quad \text{on } B_d \quad (2.26)$$

Neumann conditions:

This boundary condition is employed when the flux results from pressure-head gradient is known as a function of time. It is written as

$$-\mathbf{n} \cdot \mathbf{K} \cdot \nabla h = q_n(x_b, y_b, z_b, t) \quad \text{on } B_n, \quad (2.27)$$

Cauchy conditions:

This boundary condition is employed when the flux results from total-head gradient is known as a function of time. It can be written as

$$-\mathbf{n} \cdot (\mathbf{K} \cdot \nabla h + \mathbf{K} \cdot \nabla z) = q_c(x_b, y_b, z_b, t) \quad \text{on } B_c, \quad (2.28)$$

River Boundary Conditions:

$$-\mathbf{n} \cdot \mathbf{K} \cdot (\nabla h + \nabla z) = -\frac{K_R}{b_R}(h_R - h) \quad \text{on } B_r \quad (2.29)$$

Variable conditions:

This boundary condition is usually used for the ground surface boundary when the coupling of surface and subsurface systems is not taken into account.

(1) During precipitation periods:

$$h = h_p(x_b, y_b, z_b, t) \quad \text{on } B_v \quad (2.30)$$

or

$$-\mathbf{n} \cdot \mathbf{K} \cdot (\nabla h + \nabla z) = q_p(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (2.31)$$

(2) During non-precipitation periods

$$h = h_p(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (2.32)$$

or

$$h = h_m(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (2.33)$$

or

$$-\mathbf{n} \cdot \mathbf{K} \cdot (\nabla h + \nabla z) = q_e(x_b, y_b, z_b, t) \quad \text{on } B_v, \quad (2.34)$$

Surface/Subsurface interface variable conditions:

This boundary condition is usually used for the ground surface boundary (i.e., the interface of surface and subsurface systems) when the coupling of surface and subsurface systems is taken into consideration.

(1) During precipitation periods:

$$h = h_2(x_b, y_b, z_b, t) \quad \text{on } B_{iv} \quad (2.35)$$

or

$$-\mathbf{n} \cdot \mathbf{K} \cdot (\nabla h + \nabla z) = q_p(x_b, y_b, z_b, t) + \frac{h_2(x_b, y_b, z_b, t)}{\Delta t} \quad \text{on } B_{iv}, \quad (2.36)$$

(2) During non-precipitation periods

$$h = h_2(x_b, y_b, z_b, t) \quad \text{on } B_{iv}, \quad (2.37)$$

or

$$h = h_m(x_b, y_b, z_b, t) \quad \text{on } B_{iv}, \quad (2.38)$$

or

$$-\mathbf{n} \cdot \mathbf{K} \cdot (\nabla h + \nabla z) = q_e(x_b, y_b, z_b, t) \quad \text{on } B_{iv}, \quad (2.39)$$

where (x_b, y_b, z_b) is the spatial coordinate on the boundary; \mathbf{n} is an outward unit vector normal to the boundary; h_d , q_n , and q_c are the prescribed Dirichlet functional value [L], Neumann flux [$L^3/L^2/T$], and Cauchy flux [$L^3/L^2/T$], respectively; B_d , B_n , and B_c are the Dirichlet, Neumann, and Cauchy boundary, respectively; B_v is the variable boundary and B_{iv} is the surface/subsurface interface variable boundary; h_p is the allowed ponding depth [L] and q_p is the throughfall of precipitation [L/T], respectively, on the variable boundary; h_m is the allowed minimum pressure head [L] on the variable boundary; h_2 is water depth [L] at surface; q_e is the allowed maximum evaporation rate [$L^3/L^2/T$] on the variable boundary, which is the potential evaporation; Δt is time step size [T]; K_R is the hydraulic conductivity of the river bottom sediment layer [L/T], b_R is the thickness of the river bottom sediment layer [L], h_R is the depth of the river bottom measured from the river surface to the top of the bottom sediment layer [L], and B_r is the river boundary segment. Only one of Eqs. (2.30) through (2.34) is used at any point on the variable boundary at any time. It should be noted that when both surface and subsurface flows are simulated, the allowed ponding depth (h_p) is the actual water depth computed in the surface models (i.e., h_2 in Eqs. (2.35) through (2.37)) and the maximum infiltration is equal to the sum of throughfall of precipitation (q_p) and the average consumption rate of surface water depth during a time step.

2.4. Chemical and sediment transport in 1-D river/stream

The transport governing equations of both chemicals and sediments in 1-D river/stream system can be derived based on the conservation law of material mass [Yeh, 1983]. They can be written as follows.

Continuity equation for suspended sediments:

$$\frac{\partial(A S_n)}{\partial t} + \frac{\partial(Q S_n)}{\partial x} - \frac{\partial}{\partial x} \left[K_x A \frac{\partial S_n}{\partial x} \right] = M_n^s + M_n^{os} + (R_n - D_n)P \quad n \in [1, N_s] \quad (2.40)$$

Continuity equation for bed sediments:

$$\frac{\partial M_n}{\partial t} = D_n - R_n \quad n \in [1, N_s] \quad (2.41)$$

Continuity equation for dissolved chemicals:

$$\begin{aligned}
& \frac{\partial(AC_i^w)}{\partial t} + \frac{\partial(QC_i^w)}{\partial x} - \frac{\partial}{\partial x} \left[K_x A \frac{\partial C_i^w}{\partial x} \right] \\
& = M_i^{cw} - \lambda_i^c AC_i^w + A k_i^{ab} \left(p_i - \frac{k_i^{af}}{k_i^{ab}} C_i^w \right) + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n A \left(C_{ni}^s - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w \right) + M_i^{crw} - M_i^{ciw} + M_i^{cow} \quad (2.42) \\
& + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n P \left(C_{ni}^b - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w \right) + \sum_{m=1}^{N_r} (a_{mj}^c - b_{mj}^c) k_m^{rb} A \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \right] \quad i \in [1, N_c]
\end{aligned}$$

Continuity equation for particulate chemicals on suspended sediments:

$$\begin{aligned}
& \frac{\partial(AS_n C_{ni}^s)}{\partial t} + \frac{\partial(QS_n C_{ni}^s)}{\partial x} - \frac{\partial}{\partial x} \left[K_x A \frac{\partial(S_n C_{ni}^s)}{\partial x} \right] \\
& = M_{ni}^{cs} - \lambda_{ni}^s AS_n C_{ni}^s - k_{ni}^{sb} S_n A \left(C_{ni}^s - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w \right) + R_n B C_{ni}^b - D_n B C_{ni}^s + M_{ni}^{cos} \quad (2.43) \\
& n \in [1, N_s], i \in [1, N_c]
\end{aligned}$$

Continuity equation for particulate chemicals on bed sediments:

$$\frac{\partial(M_n C_{ni}^b)}{\partial t} = (D_n C_{ni}^s - R_n C_{ni}^b) - \lambda_{ni}^b M_n C_{ni}^b - k_{ni}^{bb} M_n \left[C_{ni}^b - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w \right] \quad n \in [1, N_s], i \in [1, N_c] \quad (2.44)$$

where

- A = River/stream cross-sectional area [L²];
- a_{mj}^c = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a reactant chemical;
- B = Top river/stream width [L];
- b_{mj}^c = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a product chemical;
- C_i^w = Cross-sectionally-averaged concentration of the i-th dissolved chemical [M/L³];
- C_i^{rw} = Concentration of the i-th dissolved chemical in rainfall [M/L³];
- C_i^{sw} = Concentration of the i-th dissolved chemical in the subsurface [M/L³];
- C_{ni}^b = Cross-sectionally-averaged particulate chemical concentration on bed sediment of the n-th fraction size [M/M];
- C_{ni}^s = Cross-sectionally-averaged particulate chemical concentration on suspended sediment of the n-th fraction size [M/M];
- D_n = Deposition rate of the n-th size fraction sediment [M/L²/T];
- I = Infiltration from river/stream to subsurface [L²/T];
- K_x = Longitudinal dispersion coefficient [L²/T];
- k_i^{ab} = Backward volatilization rate constant associated with the i-th dissolved chemical in the atmosphere [M/atm/L³/T];
- k_i^{af} = Forward volatilization rate constant associated with the i-th dissolved chemical in the

	atmosphere [1/T];
k_{ni}^{sb}	= Backward adsorption rate constant associated with the i-th particulate chemical on suspended sediment of the n-th fraction size [1/T];
k_{ni}^{sf}	= Forward adsorption rate constant associated with the i-th particulate chemical on suspended sediment of the n-th fraction size [$L^3/M/T$];
k_m^{rb}	= Backward rate constant of the m-th aqueous complexation reaction [reaction-dependent];
k_m^{rf}	= Forward rate constant of the m-th aqueous complexation reaction [reaction-dependent];
k_{ni}^{bb}	= Backward adsorption rate constant associated with the i-th particulate chemical on suspended sediment of the n-th fraction size [1/T];
k_{ni}^{bf}	= Forward adsorption rate constant associated with the i-th particulate chemical on bed sediment of the n-th fraction size [$L^3/M/T$];
M_n	= Sediment mass per unit bed area of the n-th size fraction [M/L^2];
M_n^s	= Source of the n-th size fraction sediment [$M/L/T$];
M_n^{os}	= Source of the n-th size fraction sediment from overland [$M/L/T$]; It is equal to $R_1 S_n^{os1} + R_2 S_n^{os2}$, where S_n^{os1} and S_n^{os2} are the associated suspended sediment concentration of the n-th size fraction from overland.
M_{ni}^{cs}	= Source of the i-th particulate chemical on suspended sediment of the n-th fraction size [$M/L/T$];
M_{ni}^{cos}	= Source of the i-th particulate chemical on suspended sediment of the n-th fraction size from overland [$M/L/T$]; It is equal to $R_1 S_n^{os1} C_{ni}^{os1} + R_2 S_n^{os2} C_{ni}^{os2}$, where C_{ni}^{os1} and C_{ni}^{os2} are the associated i-th particulate chemical concentration on suspended sediment of the n-th size fraction from overland.
M_i^{cw}	= Source of the i-th dissolved chemical [$M/L/T$];
M_i^{crw}	= Rainfall source of the i-th dissolved chemical [$M/L/T$]; It is equal to RC_i^{rw} if R is positive. Otherwise, it is zero.
M_i^{ciw}	= Infiltration sink of the i-th dissolved chemical [$M/L/T$]; It is equal to IC_i^w if I is positive. Otherwise, it is IC_i^{sw} representing a source from the subsurface.
M_i^{cow}	= Source of the i-th dissolved chemical from overland [$M/L/T$]; it is equal to $R_1 C_i^{ow1} + R_2 C_i^{ow2}$, where C_i^{ow1} and C_i^{ow2} are the associated i-th dissolved chemical concentrations from overland.
N_c	= Number of dissolved chemicals;
N_{rx}	= Number of aqueous complexation reactions;
N_s	= Number of sizes of sediments;
P	= Wetted perimeter [L];
p_i	= Partial pressure of the i-th dissolved chemical in the atmosphere [atm];
Q	= River/stream flow rate [L^3/T];
R	= Rainfall to river/stream [L^2/T];
R_n	= Erosion rate of the n-th size fraction sediment [$M/L^2/T$];
R_1, R_2	= Surface runoff from overland to river/stream [L^2/T]; the subscripts 1 and 2 are used to differentiate the flows through the two river/stream-overland interfaces because they usually are not the same in practice.
S_n	= Cross-sectionally-averaged sediment concentration of the n-th fraction size [M/L^3];
t	= Time [T];
x	= River/stream coordinate [L];
λ_i^c	= Combined first order degradation rate constant of the i-th dissolved chemical [1/T];
λ_{ni}^b	= Combined first order degradation rate constant of the i-th particulate chemical on bed

λ_{ni}^s = sediment of the n-th fraction size [1/T];
 Combined first order degradation rate constant of the i-th particulate chemical on suspended sediment of the n-th fraction size [1/T];

In obtaining Eqs. (2.42) through (2.44), the following reactions are considered.

(1) Aqueous complexation reactions: k_m^{rb} and k_m^{rf} as backward and forward reaction rate constants.

$$\sum_{j=1}^{N_c} a_{mj}^c \overline{C_j^w} \rightleftharpoons \sum_{j=1}^{N_c} b_{mj}^c \overline{C_j^w} \quad m \in [1, N_{rx}] \quad (2.45)$$

$$R = k_m^{rf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}} - k_m^{rb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}} \quad (2.46)$$

where R is defined as the reaction rate of the aqueous complexation reaction.

(2) Adsorption/desorption between the dissolved phase and suspended sediment: k_{ni}^{sb} and k_{ni}^{sf} as backward and forward reaction rate constants.

$$\overline{C_i^w} + \overline{S_n} \rightleftharpoons \overline{C_{ni}^s} + \overline{S_n} \quad i \in [1, N_c], n \in [1, N_s] \quad (2.47)$$

$$R = k_{ni}^{sf} S_n C_i^w - k_{ni}^{sb} S_n C_{ni}^s \quad (2.48)$$

where R is defined as the reaction rate of the adsorption reaction.

(3) Adsorption/desorption between the dissolved phase and bed sediment: k_{ni}^{bb} and k_{ni}^{bf} as backward and forward reaction rate constants.

$$\overline{C_i^w} + \overline{M_n} \rightleftharpoons \overline{C_{ni}^b} + \overline{M_n} \quad i \in [1, N_c], n \in [1, N_s] \quad (2.49)$$

$$R = k_{ni}^{bf} M_n C_i^w - k_{ni}^{bb} M_n C_{ni}^b \quad (2.50)$$

where R is defined as the reaction rate of the adsorption reaction.

(4) Volatilization between the dissolved phase and atmosphere: k_i^{ab} and k_i^{af} as backward and forward reaction rate constants.

$$\overline{C_i^w} \rightleftharpoons \overline{p_i} \quad i \in [1, N_c] \quad (2.51)$$

$$R = k_i^{af} C_i^w - k_i^{ab} p_i \quad (2.52)$$

where R is defined as the reaction rate of the volatilization reaction. In Eqs. (2.45), (2.47), (2.49), and (2.51), the overline is used to present the formula, rather than the concentration, of a chemical or a sediment.

The concentrations of all chemical species and sediments must be given initially for transient simulations. In the model, both bed sediments and particulate chemicals sorbed on the bed sediments are considered to be immobile, as described by Eqs. (2.41) and (2.44). Therefore, boundary conditions are needed for suspended sediments, dissolved chemicals, and particulate chemicals on suspended sediments. Four types of boundary conditions are taken into account as stated as follows.

Dirichlet boundary condition:

This conditions is applied when concentration is given at the boundary. That is,

$$C(x_b, t) = C_b(t) \quad (2.53)$$

where C can be the S_n , C_i^w , or $S_n C_{ni}^s$; $C_b(t)$ is a time-dependent concentration $[M/L^3]$.

Variable boundary condition:

This boundary condition is employed when the flow direction would change with time during simulations. Two cases are considered, regarding to the flow direction on the boundary.

< Case 1 > Flow is coming in from outside:

$$\left[QC(x_b, t) - AK_x \frac{\partial C(x_b, t)}{\partial x} \right] = QC_b(t) \quad (2.54)$$

< Case 2 > Flow is going out from inside:

$$-AK_x \frac{\partial C(x_b, t)}{\partial x} = 0 \quad \text{on } B_v \quad (2.55)$$

where $C_b(t)$ is a time-dependent concentration $[M/L^3]$ which is associated with the incoming flow.

Cauchy boundary condition:

This boundary condition is employed when the total material flow rate is given at the river/stream boundary. Usually, this boundary is a upstream boundary node. The conditions can be expressed as

$$n \left[QC(x_b, t) - AK_x \frac{\partial C(x_b, t)}{\partial x} \right] = Q_b^c(t) \quad (2.56)$$

where $Q_b^c(t)$ is material flow rate $[M/T]$; $n = 1$ if the boundary is a upstream boundary node, or $n = -1$ if it is a downstream boundary node.

Neumann boundary condition:

This boundary condition is used when the diffusive material flow rate is known at the river/stream boundary node. It can be written as

$$-nAK_x \frac{\partial C(x_b, t)}{\partial x} = Q_b^c(t) \quad (2.57)$$

where $Q_b^c(t)$ is material flow rate $[M/T]$.

2.5. Chemical and sediment transport in 2-D overland

The equations governing chemical and sediment transport in 2-D overland can be derived according

to the conservation law of material mass. They can be written as follows.

Continuity equation for suspended sediments:

$$\frac{\partial(hS_n)}{\partial t} + \nabla \cdot (\mathbf{q} S_n) = \nabla \cdot [h \mathbf{K} \cdot \nabla S_n] + M_n^s + (R_n - D_n) \quad n \in [1, N_s] \quad (2.58)$$

Continuity equation for bed sediments:

$$\frac{\partial M_n}{\partial t} = D_n - R_n \quad n \in [1, N_s] \quad (2.59)$$

Continuity equation for dissolved chemicals:

$$\begin{aligned} & \frac{\partial(hC_i^w)}{\partial t} + \nabla \cdot (\mathbf{q} C_i^w) \\ &= \nabla \cdot [h \mathbf{K} \cdot \nabla C_i^w] + M_i^{cw} - \lambda_i^c h C_i^w + h k_i^{ab} \left(p_i - \frac{k_i^{af}}{k_i^{ab}} C_i^w \right) + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n h \left(C_{ni}^s - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w \right) \\ &+ \sum_{n=1}^{N_s} k_{ni}^{bb} M_n \left(C_{ni}^b - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w \right) + \sum_{m=1}^{N_{rx}} (a_{mj}^c - b_{mj}^c) k_m^{rb} h \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \right] \\ &+ M_i^{crw} - M_i^{ciw} \quad i \in [1, N_c] \end{aligned} \quad (2.60)$$

Continuity equation for particulate chemical on suspended sediments:

$$\begin{aligned} & \frac{\partial(hS_n C_{ni}^s)}{\partial t} + \nabla \cdot (\mathbf{q} S_n C_{ni}^s) \\ &= \nabla \cdot [h \mathbf{K} \cdot \nabla (S_n C_{ni}^s)] + M_{ni}^{cs} - \lambda_{ni}^s h S_n C_{ni}^s - k_{ni}^{sb} S_n h \left(C_{ni}^s - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w \right) \\ &+ R_n C_{ni}^b - D_n C_{ni}^s \quad n \in [1, N_s], i \in [1, N_c] \end{aligned} \quad (2.61)$$

Continuity equation for particulate chemical on bed sediments:

$$\frac{\partial(M_n C_{ni}^b)}{\partial t} = (D_n C_{ni}^s - R_n C_{ni}^b) - \lambda_{ni}^b M_n C_{ni}^b - k_{ni}^{bb} M_n \left[C_{ni}^b - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w \right] \quad n \in [1, N_s], i \in [1, N_c] \quad (2.62)$$

where

- h = Water depth [L];
- a_{mj}^c = Stoichiometric coefficient of the j -th dissolved chemical in the m -th aqueous complexation reaction when this dissolved chemical appears as a reactant chemical;
- b_{mj}^c = Stoichiometric coefficient of the j -th dissolved chemical in the m -th aqueous complexation reaction when this dissolved chemical appears as a product chemical;
- C_i^w = Depth-averaged concentration of the i -th dissolved chemical [M/L^3];

C_i^{rw}	=	Concentration of the i-th dissolved chemical in rainfall [M/L ³];
C_i^{sw}	=	Concentration of the i-th dissolved chemical in the subsurface [M/L ³];
C_{ni}^b	=	Depth-averaged particulate chemical concentration on bed sediment of the n-th fraction size [M/M];
C_{ni}^s	=	Depth-averaged particulate chemical concentration on suspended sediment of the n-th fraction size [M/M];
D_n	=	Deposition rate of the n-th size fraction sediment [M/L ² /T];
I	=	Infiltration from overland to subsurface [L/T];
K	=	Dispersion coefficient tensor [L ² /T];
k_i^{ab}	=	Backward volatilization rate constant associated with the i-th dissolved chemical in the atmosphere [M/atm/L ³ /T];
k_i^{af}	=	Forward volatilization rate constant associated with the i-th dissolved chemical in the atmosphere [1/T];
k_{ni}^{sb}	=	Backward adsorption rate constant associated with the i-th particulate chemical on suspended sediment of the n-th fraction size [1/T];
k_{ni}^{sf}	=	Forward adsorption rate constant associated with the i-th particulate chemical on suspended sediment of the n-th fraction size [L ³ /M/T];
k_m^{rb}	=	Backward rate constant of the m-th aqueous complexation reaction [reaction-dependent];
k_m^{rf}	=	Forward rate constant of the m-th aqueous complexation reaction [reaction-dependent];
k_{ni}^{bb}	=	Backward adsorption rate constant associated with the i-th particulate chemical on suspended sediment of the n-th fraction size [1/T];
k_{ni}^{bf}	=	Forward adsorption rate constant associated with the i-th particulate chemical on bed sediment of the n-th fraction size [L ³ /M/T];
M_n	=	Sediment mass per unit bed area of the n-th size fraction [M/L ²];
M_n^s	=	Source of the n-th size fraction sediment [M/L ² /T];
M_{ni}^{cs}	=	Source of the i-th particulate chemical on suspended sediment of the n-th fraction size [M/L ² /T];
M_i^{cw}	=	Source of the i-th dissolved chemical [M/L ² /T];
M_i^{crw}	=	Rainfall source of the i-th dissolved chemical [M/L ² /T]; It is equal to rC_i^{rw} if r is positive. Otherwise, it is zero.
M_i^{ciw}	=	Infiltration sink of the i-th dissolved chemical [M/L ² /T]; It is equal to iC_i^w if i is positive. Otherwise, it is iC_i^{sw} representing a source from the subsurface.
N_c	=	Number of dissolved chemicals;
N_s	=	Number of sizes of sediments;
p_i	=	Gaseous pressure in the atmosphere associated with the i-th dissolved chemical [atm];
q	=	Flux of overland flow [L ² /T];
R	=	Rainfall to overland [L/T];
R_n	=	Erosion rate of the n-th size fraction sediment [M/L ² /T];
S_n	=	Depth-averaged sediment concentration of the n-th fraction size [M/L ³];
SS	=	External source/sink [L/t];
t	=	Time [T];
(x,y)	=	Horizontal coordinates [L];
λ_i^c	=	Combined first order degradation rate constant of the i-th dissolved chemical [1/T];
λ_{ni}^b	=	Combined first order degradation rate constant of the i-th particulate chemical on bed sediment of the n-th fraction size [1/T];
λ_{ni}^s	=	Combined first order degradation rate constant of the i-th particulate chemical on suspended sediment of the n-th fraction size [1/T];

In obtaining the above equations, the reactions described with Eqs. (2.45) through (2.52) are considered. To achieve transient simulations, the concentrations of chemicals and sediments must be provided initially. Four types of boundary conditions can be used for mobile materials, i.e., suspended sediments, dissolved chemicals, and particulate chemicals on suspended sediments. These four boundary conditions are

Dirichlet boundary condition:

This conditions is applied when concentration is given at the boundary. That is,

$$C(x_b, y_b, t) = C_b(t) \quad (2.63)$$

where C can be the S_n , C_i^w , or $S_n C_m^s$; $C_b(t)$ is a time-dependent concentration $[M/L^3]$.

Variable boundary condition:

This boundary condition is employed when the flow direction would change with time during simulations. Two cases are considered, regarding to the flow direction on the overland boundary segment.

< Case 1 > Flow is coming in from outside:

$$-\mathbf{n} \cdot [\mathbf{q} C(x_b, y_b, t) - h \mathbf{K} \cdot \nabla C(x_b, y_b, t)] = -\mathbf{n} \cdot \mathbf{q} C_b(t) \quad (2.64)$$

< Case 2 > Flow is going out from inside:

$$\mathbf{n} \cdot (-h \mathbf{K} \cdot \nabla C(x_b, y_b, t)) = 0 \quad (2.65)$$

where \mathbf{n} is the outward unit normal vector of the boundary segment; $C_b(t)$ is a time-dependent concentration $[M/L^3]$, which is associated with the incoming flow. If both 1-D river transport and 2-D overland transport are taken into account, the 1-D/2-D interface boundary is considered to be a variable boundary. In this case, Eqs. (2.64) and (2.65) are still valid but $C_b(t)$ in Eq. (2.64) is the concentration of the mobile material being considered at 1-D node corresponding to the interface boundary.

Cauchy boundary condition:

This condition is applied when the total incoming material flux is prescribed as a function of time on an overland boundary segment. It can be written as

$$-\mathbf{n} \cdot [\mathbf{q} C(x_b, y_b, t) - h \mathbf{K} \cdot \nabla C(x_b, y_b, t)] = q_b^c(t) \quad (2.66)$$

where $q_b^c(t)$ is a time-dependent Cauchy flux $[M/T/L]$

Neumann boundary condition:

This conditions is employed when the incoming diffusive material flux can be prescribed on a boundary segment. It is written as

$$-\mathbf{n} \cdot (-h \mathbf{K} \cdot \nabla C(x_b, y_b, t)) = q_b^c(t) \quad (2.67)$$

where $q_b^c(t)$ is a time-dependent Neumann flux $[M/T/L]$.

2.6. Chemical transport in 3-D subsurface

The governing equation of chemical transport in the subsurface can be derived based on the conservation law of chemical mass. Three types of chemicals are considered in the model, namely, dissolved chemicals, adsorbing sites, and adsorbed chemicals. A dissolved chemical is a chemical species existing in the aqueous phase. An adsorbing site is a chemical associated with the solid phase. Dissolved chemicals can interact with one another through aqueous complexation. They may also react with adsorbing sites to form adsorbed chemicals through adsorption. Both adsorbing sites and adsorbed chemicals are considered to be immobile. The continuity equations for the three types of chemicals can be written as follows.

(1) For dissolved chemicals:

$$\begin{aligned} & \frac{\partial(\theta C_j^w)}{\partial t} + \nabla \cdot (\mathbf{V} C_j^w) - \nabla \cdot (\theta \mathbf{D} \cdot \nabla C_j) \\ &= q C_j^{\text{in}} - \lambda_j^c \theta C_j^w - \sum_{m=1}^{N_{rx}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{\text{rf}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} - k_m^{\text{rb}} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \right] \\ & - \sum_{m=1}^{N_{rs}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{\text{sf}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{\text{sb}} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_c] \end{aligned} \quad (2.68)$$

(2) For adsorbing sites:

$$\begin{aligned} & \frac{\partial(\theta S_j)}{\partial t} \\ &= - \lambda_j^s \theta S_j - \sum_{m=1}^{N_{rs}} a_{mj}^s \theta \left[k_m^{\text{sf}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{\text{sb}} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_s] \end{aligned} \quad (2.69)$$

(3) For adsorbed chemical:

$$\begin{aligned} & \frac{\partial(\theta D_j)}{\partial t} \\ &= - \lambda_j^d \theta D_j + \sum_{m=1}^{N_{rs}} b_{mj}^d \theta \left[k_m^{\text{sf}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{\text{sb}} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_d] \end{aligned} \quad (2.70)$$

where

- a_{mj}^c = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a reactant chemical;
- b_{mj}^c = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a product chemical;
- C_i^w = Concentration of the i-th dissolved chemical [M/L³ solution];
- C_i^{in} = Concentration of the i-th dissolved chemical in the source [M/L³];
- D_i = Concentration of the i-th adsorbed chemical [M/L³ solution];
- \mathbf{D} = Dispersion coefficient tensor [L²/T];
- k_m^{sb} = Backward rate constant of the m-th adsorption reaction [reaction-dependent];

k_m^{sf}	=	Forward rate constant of the m-th adsorption reaction [reaction-dependent];
k_m^{rb}	=	Backward rate constant of the m-th aqueous complexation reaction [reaction-dependent];
k_m^{rf}	=	Forward rate constant of the m-th aqueous complexation reaction [reaction-dependent];
N_c	=	Number of dissolved chemicals;
N_d	=	Number of adsorbed chemicals;
N_s	=	Number of sizes of adsorbing sites;
N_{rx}	=	Number of aqueous complexation reactions;
N_{rxs}	=	Number of adsorption reactions;
q	=	Flow rate of source/sink [L^3 solution/ L^3 matrix/T];
S_i	=	Concentration of the i-th adsorbing site [M/L^3 solution];
t	=	Time [T];
θ	=	moisture content [L^3 solution/ L^3 matrix];
λ_i^c	=	Combined first order degradation rate constant of the i-th dissolved chemical [1/T];
λ_i^d	=	Combined first order degradation rate constant of the i-th adsorbed chemical [1/T];
λ_i^s	=	Combined first order degradation rate constant of the i-th adsorbing site [1/T].

The dispersion coefficient tensor \mathbf{D} in Eq. (2.63) is given by

$$\theta \mathbf{D} = a_T |\mathbf{V}| \delta + (a_L - a_T) \mathbf{V} \mathbf{V} / |\mathbf{V}| + \theta a_m \tau \delta \quad (2.71)$$

where $|\mathbf{V}|$ is the magnitude of \mathbf{V} [L/T], δ is the Kronecker delta tensor, a_T is lateral dispersivity [L], a_L is the longitudinal dispersivity [L], a_m is the molecular diffusion coefficient [L^2/T], and τ is the tortuosity.

In deriving Eqs. (2.68) through (2.70), the following reactions are taken into account.

(1) Aqueous complexation reactions: k_m^{rb} and k_m^{rf} as backward and forward reaction rate constants.

$$\sum_{j=1}^{N_c} a_{mj}^c \overline{C_j^w} \rightleftharpoons \sum_{j=1}^{N_c} b_{mj}^c \overline{C_j^w} \quad m \in [1, N_{rx}] \quad (2.72)$$

$$R = k_m^{rf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} - k_m^{rb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \quad (2.73)$$

where R is defined as the reaction rate of the aqueous complexation reaction.

(2) Adsorption/desorption between the dissolved phase and adsorbing sites: k_{ni}^{sb} and k_{ni}^{sf} as backward and forward reaction rate constants.

$$\sum_{j=1}^{N_c} a_{mj}^c \overline{C_j^w} + \sum_{j=1}^{N_s} a_{mj}^s \overline{S_j} \rightleftharpoons \sum_{j=1}^{N_d} b_{mj}^d \overline{D_j} + \sum_{j=1}^{N_c} b_{mj}^c \overline{C_j^w} \quad m \in [1, N_{rxs}] \quad (2.74)$$

$$R = k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \quad (2.75)$$

where R is defined as the reaction rate of the adsorption reaction.

The initial and boundary conditions used to solve the transport governing equations are stated below.

Initial Conditions:

$$C_j^w = C_j^{\text{initial}}(x,y,z) \quad \text{in } R \quad (2.76)$$

$$D_j = D_j^{\text{initial}}(x,y,z) \quad \text{in } R \quad (2.77)$$

$$S_j = S_j^{\text{initial}}(x,y,z) \quad \text{in } R \quad (2.78)$$

Prescribed Concentration (Dirichlet) Boundary Conditions:

$$C_j^w = C_j^{\text{Dirichlet}}(x_b, y_b, z_b, t) \quad \text{on } B_d \quad (2.79)$$

Variable boundary Conditions:

$$\mathbf{n} \cdot (\mathbf{V} C_j^w - \theta \mathbf{D} \cdot \nabla C_j^w) = \mathbf{n} \cdot \mathbf{V} C_u^{\text{Variable}}(x_b, y_b, z_b, t) \quad \text{if } \mathbf{n} \cdot \mathbf{V} \leq 0 \quad (2.80)$$

$$\mathbf{n} \cdot (-\theta \mathbf{D} \cdot \nabla C_j^w) = 0 \quad \text{if } \mathbf{n} \cdot \mathbf{V} > 0 \quad (2.81)$$

Cauchy Boundary Conditions:

$$\mathbf{n} \cdot (\mathbf{V} C_j^w - \theta \mathbf{D} \cdot \nabla C_j^w) = q_j^{\text{Cauchy}}(x_b, y_b, z_b, t) \quad \text{on } B_c \quad (2.82)$$

Neumann Boundary Conditions:

$$\mathbf{n} \cdot (-\theta \mathbf{D} \cdot \nabla C_j^w) = q_j^{\text{Neumann}}(x_b, y_b, z_b, t) \quad \text{on } B_n \quad (2.83)$$

where C_j^{initial} , D_j^{initial} , and S_j^{initial} are the initial concentrations of the j-th dissolved chemical, the j-th adsorbed chemical, and the j-th adsorbing sites, respectively $[M/L^3]$; R is the region of interest; (x_b, y_b, z_b) is the spatial coordinate on the boundary; \mathbf{n} is an outward unit vector normal to the boundary; $C_j^{\text{Dirichlet}}$ and C_j^{Variable} are the prescribed concentration of the j-th dissolved chemical on the Dirichlet boundary and the specified concentration of water through the variable boundary, respectively $[M/L^3]$; B_d and B_v are the Dirichlet and variable boundaries respectively; q_j^{Cauchy} and q_j^{Neumann} are the prescribed total flux and gradient flux of the j-th dissolved chemical through the Cauchy and Neumann boundaries B_c and B_n , respectively $[M/L^2/T]$. It is noted that when both surface and subsurface transport are simulated, C_j^{Variable} is the concentration of the j-th dissolved chemical associated with the corresponding surface nodes if it is not dry at that node. If the corresponding surface node is dry, however, the infiltration is equal to the throughfall and C_j^{Variable} is the concentration of the j-th dissolved chemical in the throughfall.

Section 3. NUMERICAL APPROACHES

In this section, we present the numerical approaches employed to solve the governing equations of flow and transport given in the previous section. In the model, transport is assumed not to influence flow and a one-time-lag approach is taken to deal with the interaction between surface and subsurface systems. Three time scales are considered in the model. They are (1) for 3-D subsurface flow, (2) for 3-D subsurface transport and 2-D overland flow/transport, and (3) for 1-D river/stream flow/transport. In general, a 3-D flow time step may include several 2-D flow time steps and a 2-D flow time step can cover many 1-D flow time steps. The time scale for 3-D subsurface transport is set to be the same as that for 2-D overland flow/transport because kinetic chemical reactions are taken into account. During each 3-D flow time step, we solve 3-D subsurface flow by employing the updated 2-D flow conditions to achieve the surface/subsurface interface boundary conditions and determine the infiltration/seepage for 2-D flow computation included in this 3-D flow time step. During each 2-D flow time step, we first solve 3-D reactive chemical transport with the updated 2-D transport result (i.e., at the previous time) used for implementing variable boundary conditions on the interface boundary and determine the dissolve chemical flux through the surface/subsurface interface. This flux is actually the source/sink to 2-D dissolve chemical transport through infiltration/seepage. Then we solve 2-D flow equations to determine the water stage/depth and velocity of overland flow. Finally, we solve 2-D reactive chemical transport equations for the distribution of dissolved chemicals, sediments, and particulate chemicals. Within a 1-D flow time step, the river/stream flow equations are solved first and the 1-D transport equations are solved by using the newly-computed flow results. The interaction between 1-D river/stream and 2-D overland flow/transport is taken into account by using the updated computational results. Depth or stage difference-dependent fluxes are employed to determine the flow through this 1-D/2-D interface.

3.1. Solving the 1-D river/stream flow equations

As mentioned earlier in this report, we desire to implement a hybrid model to accurately simulate surface water flow under a wide range of physical conditions though it is still under investigation and further study is required. In our investigation to date, we would apply the method of characteristics to solve the dynamical wave model and would use the Lagrangian approach to solve both the diffusion wave and the kinematic wave models in the hybrid model that is composed of the aforementioned three wave models. In this and the next subsections, we will present the numerical approaches used in the method of characteristics and the Lagrangian approach for solving the 1-D river/stream flow and 2-D overland flow equations, respectively. In either approach, the Picard method is employed to deal with the nonlinearity.

3.1.1. Method of characteristics for 1-D dynamic wave model

Recall Eqs. (2.1) and (2.2),

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = S_s + S_R - S_1 + S_1 + S_2 \quad (3.1)$$

$$\frac{\partial Q}{\partial t} + \frac{\partial uQ}{\partial x} = -gA \frac{\partial(Z_0 + h)}{\partial x} + \frac{\partial F_x}{\partial x} + u^1 S_R - u^1 S_1 + u^{Y1} S_1 + u^{Y2} S_2 + \frac{T^s - T^b}{\rho} \quad (3.2)$$

We also have

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = B_t \frac{\partial h}{\partial t} + \frac{\partial(uhB_a)}{\partial x} \quad (3.3)$$

$$\frac{\partial B_a}{\partial x} = \frac{\partial B_a^*}{\partial x} + \frac{\partial B_a^*}{\partial h} \frac{\partial h}{\partial x} \quad (3.4)$$

$$\frac{\partial A}{\partial t} = B_t \frac{\partial h}{\partial t} = \left[B_a^* + h \frac{\partial B_a^*}{\partial h} \right] \frac{\partial h}{\partial t} \quad (3.5)$$

and assume

$$\frac{\partial F_x}{\partial x} = \frac{\partial}{\partial x} \left[v A \frac{\partial u}{\partial x} \right] = \frac{\partial}{\partial x} \left[v B_a h \frac{\partial u}{\partial x} \right] \quad (3.6)$$

where v is the eddy viscosity coefficient [L^2/T]; $B_t(x,t)$ ($= B_t^*(x,h(x,t))$) is the top river/stream width [L]; $B_a(x,t)$ ($= B_a^*(x,h(x,t))$) is the average river/stream width [L]. Thus, Eqs. (3.1) and (3.2) can be rewritten as follows after letting $H = h + Z_0$ and some mathematical manipulation.

$$\frac{\partial H}{\partial t} + u \frac{\partial H}{\partial x} + \frac{h B_a}{B_t} \frac{\partial u}{\partial x} = \frac{1}{B_t} (S_s + S_R - S_1 + S_1 + S_2) - \frac{u h}{B_t} \frac{\partial B_a^*}{\partial x} + u \frac{\partial Z_0}{\partial x} \quad (3.7)$$

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + g \frac{\partial H}{\partial x} &= \frac{1}{h B_a} \frac{\partial}{\partial x} \left[v B_a h \frac{\partial u}{\partial x} \right] \\ &+ \frac{1}{h B_a} \left[-u S_s + (u^r - u) S_R - (u^i - u) S_1 + (u^{Y1} - u) S_1 + (u^{Y2} - u) S_2 + \frac{T^s - T^b}{\rho} \right] \end{aligned} \quad (3.8)$$

Thus, Eqs. (3.7) and (3.8) can be written in matrix form as

$$\frac{\partial E}{\partial t} + A \frac{\partial E}{\partial x} = R \quad (3.9)$$

where

$$E = \{ H \ u \}^T \quad (3.10)$$

$$A = \begin{bmatrix} u & \frac{h B_a}{B_t} \\ g & u \end{bmatrix} \quad (3.11)$$

and

$$R = \{ R_1 \ R_2 \}^T \quad (3.12)$$

in which

$$R_1 = \frac{1}{B_t} (S_S + S_R - S_I + S_1 + S_2) - \frac{uh}{B_t} \frac{\partial B_a^*}{\partial x} + u \frac{\partial Z_0}{\partial x} \quad (3.13)$$

$$R_2 = \frac{1}{hB_a} \frac{\partial}{\partial x} \left[v B_a h \frac{\partial u}{\partial x} \right] + \frac{1}{hB_a} \left[-u S_S + (u^r - u) S_R - (u^i - u) S_I + (u^{Y1} - u) S_1 + (u^{Y2} - u) S_2 + \frac{T^s - T^b}{\rho} \right] \quad (3.14)$$

Eq. (3.9) can be written as

$$\frac{\partial E}{\partial t} + A^d \frac{\partial E}{\partial x} = RJ + RD \quad (3.15)$$

where

$$A^d = \begin{bmatrix} u & 0 \\ 0 & u \end{bmatrix} \quad (3.16)$$

and

$$RD = \begin{Bmatrix} RD_1 \\ RD_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ \frac{1}{hB_a} \frac{\partial}{\partial x} \left(hB_a v \frac{\partial u}{\partial x} \right) \end{Bmatrix} \quad (3.17)$$

$$RJ = \begin{Bmatrix} RJ_1 \\ RJ_2 \end{Bmatrix} = \begin{Bmatrix} R_1 - \frac{hB_a}{B_t} \frac{\partial u}{\partial x} \\ R_2 - RD_2 - g \frac{\partial H}{\partial x} \end{Bmatrix} \quad (3.18)$$

Eq. (3.15) can be further written as

$$\frac{DE}{Dt} = RJ + RD \quad (3.19)$$

where

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A^d \frac{\partial E}{\partial x} \quad (3.20)$$

Let E^* be the solution of

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A^d \frac{\partial E}{\partial x} = RJ \quad (3.21)$$

We have, from Eq. (3.19)

$$\frac{E - E^p}{\Delta t} = RJ + RD \quad (3.22)$$

where E^p represents the Lagrangian value of E . From Eq. (3.21)

$$\frac{E^* - E^p}{\Delta t} = RJ \quad (3.23)$$

Subtracting Eq. (3.23) from Eq. (3.22) yields

$$\frac{E - E^*}{\Delta t} = RD \quad (3.24)$$

Based on the above, we mean to solve Eq. (3.21) for E^* at first and solve Eq. (3.24) for E based on E^* . Eq. (3.21) is solved by the method of characteristics as follows.

Eq. (3.21) can be written as

$$\frac{\partial E}{\partial t} + A \frac{\partial E}{\partial x} = RI \quad (3.25)$$

where

$$RJ = \begin{Bmatrix} RI_1 \\ RI_2 \end{Bmatrix} = \begin{Bmatrix} R_1 \\ R_2 - RD_2 \end{Bmatrix} \quad (3.26)$$

The eigenvalues and eigenvectors of A are

$$\lambda_1 = u + \sqrt{\frac{ghB_a}{B_t}} \quad e_1 = \left\{ \frac{1}{2} \sqrt{\frac{hB_a}{gB_t}} \quad \frac{1}{2} \right\}^T \quad (3.27)$$

$$\lambda_2 = u - \sqrt{\frac{ghB_a}{B_t}} \quad e_2 = \left\{ -\frac{1}{2} \sqrt{\frac{hB_a}{gB_t}} \quad \frac{1}{2} \right\}^T \quad (3.28)$$

Now, we define

$$L = \begin{bmatrix} \frac{c}{2g} & -\frac{c}{2g} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \quad (3.29)$$

Thus

$$L^{-1} = \begin{bmatrix} \frac{g}{c} & 1 \\ -\frac{g}{c} & 1 \end{bmatrix} \quad (3.30)$$

Set

$$\partial W = L^{-1} \partial E = \begin{bmatrix} \frac{g}{c} & 1 \\ -\frac{g}{c} & 1 \end{bmatrix} \begin{Bmatrix} \partial H \\ \partial u \end{Bmatrix} \quad (3.31)$$

Multiplying both side of Eq. (3.25) by L^{-1} yields

$$L^{-1} \frac{\partial E}{\partial t} + L^{-1} A L L^{-1} \frac{\partial E}{\partial x} = L^{-1} R I \quad (3.32)$$

or

$$\frac{\partial W}{\partial t} + \begin{bmatrix} u+c & 0 \\ 0 & u-c \end{bmatrix} \frac{\partial W}{\partial x} = L^{-1} R I \quad (3.33)$$

or

$$\frac{DW}{Dt} = L^{-1} R I \quad (3.34)$$

where

$$c = \sqrt{\frac{ghB_a}{B_t}} \quad (3.35)$$

Eq. (3.34) can be discretized, in time, as follows.

$$\frac{g}{c} \frac{H^{n+1} - H_1^*}{\Delta \tau_1} + \frac{u^{n+1} - u_1^*}{\Delta \tau_1} = \frac{g}{c} R I_1 + R I_2 \quad (3.36)$$

$$\frac{-g}{c} \frac{H^{n+1} - H_2^*}{\Delta \tau_2} + \frac{u^{n+1} - u_2^*}{\Delta \tau_2} = \frac{-g}{c} R I_1 + R I_2 \quad (3.37)$$

where H_1^* , u_1^* , and $\Delta \tau_1$ are determined by backward tracking along the first characteristic; H_2^* , u_2^* , and $\Delta \tau_2$ are determined by backward tracking along the second characteristic.

And

$$H_1^* = a_1 H_{k1}^{n+1} + a_2 H_{k2}^{n+1} + a_3 \quad (3.38)$$

$$u_1^* = a_1 u_{k1}^{n+1} + a_2 u_{k2}^{n+1} + a_4 \quad (3.39)$$

$$H_2^* = b_1 H_{j1}^{n+1} + b_2 H_{j2}^{n+1} + b_3 \quad (3.40)$$

$$u_2^* = b_1 u_{j1}^{n+1} + b_2 u_{j2}^{n+1} + b_4 \quad (3.41)$$

in which k_1 and k_2 are nodes of the element that the backward tracking, along the first characteristic, stops in; j_1 and j_2 are nodes of the element that the backward tracking, along the second characteristic, stops in. (see the above figure)

Note: 1. a_1 , a_2 , b_1 , and b_2 are within the range of $[0,1]$.
2. We may use two given parameters to determine where to stop in the backward tracking: one is for controlling tracking time and the other one is for controlling tracking distance.

Multiplying Eqs. (3.36) and (3.37) with cross-sectional area yields

$$\begin{aligned} & \frac{ghB_a}{c\Delta\tau_1}(H-H_1^*) + \frac{hB_a}{\Delta\tau_1}(u-u_1^*) + hB_a \left[\frac{c}{B_t} \frac{\partial B_a^*}{\partial x} - \frac{g}{c} \frac{\partial Z_0}{\partial x} \right] u + (Ph\kappa + S_S + S_R - S_I + S_1 + S_2)u \\ & = \frac{ghB_a}{cB_t}(S_S + S_R - S_I + S_1 + S_2) + (u^r S_R - u^i S_I + u^{Y1} S_1 + u^{Y2} S_2) + \frac{B_t \tau^s}{\rho} + \frac{\partial}{\partial x} \left(v h B_a \frac{\partial u}{\partial x} \right) \end{aligned} \quad (3.42)$$

$$\begin{aligned} & -\frac{ghB_a}{c\Delta\tau_2}(H-H_2^*) + \frac{hB_a}{\Delta\tau_2}(u-u_2^*) - hB_a \left[\frac{c}{B_t} \frac{\partial B_a^*}{\partial x} - \frac{g}{c} \frac{\partial Z_0}{\partial x} \right] u + (Ph\kappa + S_S + S_R - S_I + S_1 + S_2)u \\ & = -\frac{ghB_a}{cB_t}(S_S + S_R - S_I + S_1 + S_2) + (u^r S_R - u^i S_I + u^{Y1} S_1 + u^{Y2} S_2) + \frac{B_t \tau^s}{\rho} + \frac{\partial}{\partial x} \left(v h B_a \frac{\partial u}{\partial x} \right) \end{aligned} \quad (3.43)$$

In obtaining Eqs. (3.42) and (3.43), the following relationships have been employed.

$$\frac{T^b}{\rho} = Ph\kappa u \quad (3.44)$$

$$\frac{T^s}{\rho} = \frac{B_t \tau^s}{\rho} \quad (3.45)$$

When H_1^* , u_1^* , H_2^* , and u_2^* are determined explicitly by using the spatial reachout option in backward tracking (i.e., track backward all the way to the previous time), Eqs. (3.42) and (3.43) can be solved for (H^*, u^*) node by node as follows.

Eqs. (3.42) and (3.43), after multiplied by $\Delta\tau_1$ and $\Delta\tau_2$, respectively, can be written as

$$a_{11}H + a_{12}u = b_1 \quad (3.46)$$

$$a_{21}H + a_{22}u = b_2 \quad (3.47)$$

where

$$a_{11} = cB_a \quad (3.48)$$

$$a_{22} = hB_a \left[1 + \left(\frac{c}{B_t} \frac{\partial B_a^*}{\partial x} - \frac{g}{c} \frac{\partial Z_0}{\partial x} \right) \Delta\tau_1 \right] + (Ph\kappa + S_S + S_R - S_I + S_1 + S_2)\Delta\tau_1 \quad (3.49)$$

$$b_1 = cB_a H_1^* + hB_a u_1^* + \frac{cB_a \Delta\tau_1}{B_t} (S_S + S_R - S_1 + S_1 + S_2) + \Delta\tau_1 (u^r S_R - u^i S_1 + u^{Y1} S_1 + u^{Y2} S_2) + \frac{B_t \tau^s \Delta\tau_1}{\rho} \quad (3.50)$$

$$a_{21} = -cB_a \quad (3.51)$$

$$a_{22} = hB_a \left[1 - \left(\frac{c}{B_t} \frac{\partial B_a^*}{\partial x} - \frac{g}{c} \frac{\partial Z_0}{\partial x} \right) \Delta\tau_2 \right] + (Ph\kappa + S_S + S_R - S_1 + S_1 + S_2) \Delta\tau_2 \quad (3.52)$$

$$b_2 = -cB_a H_2^* + hB_a u_2^* - \frac{cB_a \Delta\tau_2}{B_t} (S_S + S_R - S_1 + S_1 + S_2) + \Delta\tau_2 (u^r S_R - u^i S_1 + u^{Y1} S_1 + u^{Y2} S_2) + \frac{B_t \tau^s \Delta\tau_2}{\rho} \quad (3.53)$$

Therefore, we solve Eqs. (3.46) and (3.47) for H^* and u^* . Now, we can solve Eq. (3.24) as follows. Eq. (3.24) can be written in details as

$$\frac{H - H^*}{\Delta t} = 0 \quad (3.54)$$

$$\frac{hB_a (u - u^*)}{\Delta t} = \frac{\partial}{\partial x} \left(v h B_a \frac{\partial u}{\partial x} \right) \quad (3.55)$$

Eq. (3.54) gives that $H = H^*$, while Eq. (3.55) can be discretized, in the finite element method, as

$$\frac{hB_a}{\Delta t} [QA] \{u\} + [QD] \{u\} = \{QR\} + \{BQ\} \quad (3.56)$$

where

$$QA_{ij} = \sum_{e \in M_e} \int_{R_e} N_\alpha^e N_\beta^e dR \quad (3.57)$$

$$QD_{ij} = \sum_{e \in M_e} \int_{R_e} \nabla N_\alpha^e h v B_a \nabla N_\beta^e dR \quad (3.58)$$

$$QR_i = \sum_{e \in M_e} \int_{R_e} N_\alpha^e \frac{hB_a u^*}{\Delta t} dR \quad (3.59)$$

$$BQ_i = \sum_{e \in M_e} \int_{B_e} N_\alpha^e n h B_a \frac{\partial u}{\partial x} dB \quad (3.60)$$

in Eq. (3.60), $n = -1$ for upstream boundary nodes while $n = 1$ for downstream boundary nodes.

In solving Eqs. (3.42) and (3.43) at boundary nodes, boundary conditions are implemented as follows. A boundary node can be either an closed or an open (flow-through) boundary. In the former case, nothing is specified and velocity at the node is set to zero automatically in the computer code. While in the latter case, H , and u of the approaching flow, with respect to the characteristic ongoing direction, must be given at the boundary nodes. Some details are given for both cases below.

< Case 1 > Closed boundaries:

If the closed boundary is located at the downstream end, only sub-critical flow can happen because the velocity is zero. Under this condition, one characteristic comes from the outside of the domain and the other one is from the inside. The equation associated with the characteristic from outside will be replaced by $u = 0$, while the other (either Eq. (3.40) or (3.41)) is used for the other characteristic. On the other hand, if the closed boundary is located at the upstream end, either sub-critical or super-critical flow can occur. If the flow is sub-critical, again, the equation associated with the characteristic from outside will be replaced by $u = 0$, while the other (either Eq. (3.40) or (3.41)) is used for the other characteristic. If the flow is super-critical then both u and h are set to zero.

< Case 2 > Open boundaries:

In this case, three types of boundary conditions can be given for sub-critical flow when the propagation direction of a characteristic is inward to the domain of interest and are described below.

(1) Given time-dependent flow rate, $Q(t)$: (used for upstream open boundaries)

$$\mathbf{n} \cdot \mathbf{u} = \frac{Q}{hB_a} = \frac{Q}{A} \quad (3.61)$$

(2) Given time-dependent water stage, $H_b(t)$: (used for either upstream or downstream open boundaries)

$$H = H_b \quad (3.62)$$

(3) Given rating water depth-dependent flow rate, $Q(h)$: (used for natural downstream open boundaries only)

$$\mathbf{n} \cdot \mathbf{u} = \frac{Q}{hB_a} = \frac{Q}{A} \quad (3.63)$$

On the other hand, for super-critical flow either no boundary conditions is required when the open boundary is located downstream, or both u and h must be prescribed when the open boundary is located upstream.

3.1.2. The Lagrangian approach for both 1-D diffusion and 1-D kinematic wave models

Since the kinematic wave model can be considered to be a simplified form from a mathematical point of view, we just demonstrate how the diffusion wave equations are solved with the Lagranging approach in the following. Recall Eqs. (2.1) and (2.3)

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = S_s + S_R - S_I + S_1 + S_2 \quad (3.64)$$

$$u = \frac{-1}{n} \left[\frac{R}{1 + (\nabla Z_0)^2} \right]^{2/3} \frac{1}{(\nabla(Z_0 + h))^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \quad (3.65)$$

Eq. (3.64) can be further written as

$$B_t \frac{\partial h}{\partial t} + \frac{\partial(uhB_a)}{\partial x} = S_s + S_R - S_I + S_1 + S_2 \quad (3.66)$$

Substituting Eq.(3.65) into the second term on the left side of Eq. (3.66) yields

$$\frac{\partial uhB_a}{\partial x} = uB_a \frac{\partial h}{\partial x} + uh \frac{\partial B_a}{\partial x} + hB_a \frac{\partial u}{\partial x} = \left(uB_a + uh \frac{\partial B^*}{\partial h} + hB_a \frac{2}{3} \frac{u}{R} \frac{\partial R^*}{\partial h} \right) \frac{\partial h}{\partial x} + S \quad (3.67)$$

where

$$\begin{aligned} S = & \frac{-hB_a}{n} \frac{R^{2/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{1}{(\nabla(Z_0 + h))^{1/2}} \frac{\partial^2(Z_0 + h)}{\partial x^2} + \frac{hB_a}{n^2} \frac{R^{2/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{1}{(\nabla Z_0)^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \frac{\partial n}{\partial x} \\ & + \frac{-hB_a}{n} \frac{R^{2/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{\partial Z_0}{\partial x} \frac{-1}{4} \left[\left(\frac{\partial(Z_0 + h)}{\partial x} \right)^2 \right]^{-5/4} 2 \left[\frac{\partial(Z_0 + h)}{\partial x} \frac{\partial^2(Z_0 + h)}{\partial x^2} \right] \\ & + \frac{-hB_a}{n} \left[\frac{1}{1 + (\nabla Z_0)^2} \right]^{2/3} \frac{1}{(\nabla(Z_0 + h))^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \frac{2}{3} R^{-1/3} \frac{\partial R^*}{\partial x} \\ & + \frac{-hB_a}{n} \frac{R^{2/3}}{(\nabla(Z_0 + h))^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \frac{-2}{3} [1 + (\nabla Z_0)^2]^{-5/3} 2 \left[\frac{\partial Z_0}{\partial x} \frac{\partial^2 Z_0}{\partial x^2} \right] + hu \frac{\partial B_a^*}{\partial x} \end{aligned} \quad (3.68)$$

Therefore, Eq. (3.66) can be written as

$$B_t \frac{\partial h}{\partial t} + \left(uB_a + uh \frac{\partial B^*}{\partial h} + hB_a \frac{2}{3} \frac{u}{R} \frac{\partial R^*}{\partial h} \right) \frac{\partial h}{\partial x} = S_s + S_R - S_I + S_1 + S_2 - S \quad (3.69)$$

Eq. (3.69) can be further written as

$$B_t \frac{Dh}{Dt} = S_s + S_R - S_I + S_1 + S_2 - S \quad (3.70)$$

where the following characteristic equation applies.

$$\frac{dx}{dt} = \frac{uB_a + uh \frac{\partial B^*}{\partial h} + hB_a \frac{2}{3} \frac{u}{R} \frac{\partial R^*}{\partial h}}{B_t} \quad (3.71)$$

Hence the solution to Eq. (3.69) is

$$h(x,t) = h(x_0,0) + (S_s + S_R - S_1 + S_1 + S_2 - S)t \quad (3.72)$$

in which

$$x - x_0 = \int_0^t \frac{u B_a + u h \frac{\partial B^*}{\partial h} + h B_a \frac{2}{3} \frac{u}{R} \frac{\partial R^*}{\partial h}}{B_t} dt \quad (3.73)$$

A nonlinear iteration loop with the Picard method implemented is used to solve Eqs. (3.7) and (3.8) in the dynamic wave model or to solve Eqs. (3.64) and (3.65) in the diffusion wave model during each time step.

3.1.3. Computation of water budget at junctions

In the model, a junction is considered to be a reservoir and water budget is used to determine the water stage there. Thus, the governing equation to compute water stage at a junction can be written as

$$\frac{dV_j}{dt} = \sum_{i=1}^{ncr} Q_i \quad (3.74)$$

where V_j is the volume of water at the junction [L^3]; Q_i is the flow rate associated with the junction's i -th connected river/stream reach [L^3/T]; ncr is the number of river/stream reaches that is connected to the junction. Since V_j can be expressed as a function of water depth at the junction, the stage at the junction can be determined once V_j is computed. In the model, Eq. (3.74) is solved implicitly (i.e., within the nonlinear iteration loop).

3.2. Solving the 2-D overland flow equations

3.2.1. Method of characteristics for 2-D dynamic wave model

Recall Eqs. (2.9) through (2.11)

$$\frac{\partial h}{\partial t} + \frac{\partial u h}{\partial x} + \frac{\partial v h}{\partial y} = SS + R - I \quad (3.75)$$

$$\frac{\partial u h}{\partial t} + \frac{\partial u^2 h}{\partial x} + \frac{\partial u v h}{\partial y} = -gh \frac{\partial(Z_0 + h)}{\partial x} + \frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y} + (u^r R - u^i I) + \frac{\tau_x^s - \tau_x^b}{\rho} \quad (3.76)$$

$$\frac{\partial v h}{\partial t} + \frac{\partial u v h}{\partial x} + \frac{\partial v^2 h}{\partial y} = -gh \frac{\partial(Z_0 + h)}{\partial y} + \frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y} + (v^r R - v^i I) + \frac{\tau_y^s - \tau_y^b}{\rho} \quad (3.77)$$

Let $H = h + Z_0$, then Eqs. (3.75) through (3.77) can be written as follows after mathematical manipulation.

$$\frac{\partial H}{\partial t} + u \frac{\partial H}{\partial x} + h \frac{\partial u}{\partial x} + v \frac{\partial H}{\partial y} + h \frac{\partial v}{\partial y} = (SS + R - I) + u \frac{\partial Z_0}{\partial x} + v \frac{\partial Z_0}{\partial y} \quad (3.78)$$

$$\frac{\partial u}{\partial t} + g \frac{\partial H}{\partial x} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \frac{1}{h} \left[\frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y} \right] + \frac{(u^r - u)R - (u^i - u)I}{h} + \frac{\tau_x^s - \tau_x^b}{h\rho} - \frac{SS u}{h} \quad (3.79)$$

$$\frac{\partial v}{\partial t} + g \frac{\partial H}{\partial y} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \frac{1}{h} \left[\frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y} \right] + \frac{(v^r - v)R - (v^i - v)I}{h} + \frac{\tau_y^s - \tau_y^b}{h\rho} - \frac{SS v}{h} \quad (3.80)$$

Thus, Eqs. (3.78) through (3.80) can be written in matrix form as

$$\frac{\partial E}{\partial t} + A_x \frac{\partial E}{\partial x} + A_y \frac{\partial E}{\partial y} = R \quad (3.81)$$

where

$$E = \{H \ u \ v\}^T \quad (3.82)$$

$$A_x = \begin{bmatrix} u & h & 0 \\ g & u & 0 \\ 0 & 0 & u \end{bmatrix} \quad A_y = \begin{bmatrix} v & 0 & h \\ 0 & v & 0 \\ g & 0 & v \end{bmatrix} \quad (3.83)$$

and

$$R = \begin{Bmatrix} R_1 \\ R_2 \\ R_3 \end{Bmatrix} = \begin{Bmatrix} SS + R - I + u \frac{\partial Z_0}{\partial x} + v \frac{\partial Z_0}{\partial y} \\ \frac{1}{h} \left[\frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y} \right] + \frac{(u^r - u)R - (u^i - u)I}{h} + \frac{\tau_x^s - \tau_x^b}{h\rho} - \frac{SS u}{h} \\ \frac{1}{h} \left[\frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y} \right] + \frac{(v^r - v)R - (v^i - v)I}{h} + \frac{\tau_y^s - \tau_y^b}{h\rho} - \frac{SS v}{h} \end{Bmatrix} \quad (3.84)$$

By using the splitting strategy mentioned in Section 3.1.1, Eq. (3.81) can be written as

$$\frac{\partial E}{\partial t} + A_x^d \frac{\partial E}{\partial x} + A_y^d \frac{\partial E}{\partial y} = RJ + RD \quad (3.85)$$

where

$$A_x^d = \begin{bmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u \end{bmatrix} \quad A_y^d = \begin{bmatrix} v & 0 & 0 \\ 0 & v & 0 \\ 0 & 0 & v \end{bmatrix} \quad (3.86)$$

and

$$RD = \begin{Bmatrix} RD_1 \\ RD_2 \\ RD_3 \end{Bmatrix} = \begin{Bmatrix} 0 \\ \frac{1}{h} \left[\frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y} \right] \\ \frac{1}{h} \left[\frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y} \right] \end{Bmatrix} \quad (3.87)$$

$$RJ = \begin{Bmatrix} RJ_1 \\ RJ_2 \\ RJ_3 \end{Bmatrix} = \begin{Bmatrix} R_1 - h \frac{\partial u}{\partial x} - h \frac{\partial v}{\partial y} \\ R_2 - RD_2 - g \frac{\partial H}{\partial x} \\ R_3 - RD_3 - g \frac{\partial H}{\partial y} \end{Bmatrix} \quad (3.88)$$

Eq. (3.85) can be further written as

$$\frac{DE}{Dt} = RJ + RD \quad (3.89)$$

where

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A_x^d \frac{\partial E}{\partial x} + A_y^d \frac{\partial E}{\partial y} \quad (3.90)$$

Let $E^{\#}$ be the solution of

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A_x^d \frac{\partial E}{\partial x} + A_y^d \frac{\partial E}{\partial y} = RJ \quad (3.91)$$

we have, from Eq. (3.89)

$$\frac{E - E^p}{\Delta t} = RJ + RD \quad (3.92)$$

where E^p represents the Lagrangian value of E . From Eq. (3.91)

$$\frac{E^{\#} - E^p}{\Delta t} = RJ \quad (3.93)$$

Subtracting Eq. (3.93) from Eq. (3.92) yields

$$\frac{E - E^{\#}}{\Delta t} = RD \quad (3.94)$$

Based on the above, we mean to solve Eq. (3.93) for $E^{\#}$ at first and solve Eq. (3.94) for E based on $E^{\#}$. Eq. (3.93) is to be solved by the method of characteristics and can be written, in details, as follows. Eq. (3.93) can be written as

$$\frac{\partial E}{\partial t} + A_x \frac{\partial E}{\partial x} + A_y \frac{\partial E}{\partial y} = RI \quad (3.95)$$

where

$$RI = \begin{Bmatrix} RI_1 \\ RI_2 \\ RI_3 \end{Bmatrix} = \begin{Bmatrix} R_1 \\ R_2 - RD_2 \\ R_3 - RD_3 \end{Bmatrix} \quad (3.96)$$

Let

$$A \cdot k = A_x k_x + A_y k_y = \begin{bmatrix} uk_x + vk_y & hk_x & hk_y \\ gk_x & uk_x + vk_y & 0 \\ gk_y & 0 & uk_x + vk_y \end{bmatrix} \quad (3.97)$$

the associated eigenvalues and eigenvectors are

$$\lambda_1 = uk_x + vk_y \quad e_1 = \{0 \quad k_y \quad -k_x\}^T \quad (3.98)$$

$$\lambda_2 = uk_x + vk_y + \sqrt{gh} \quad e_2 = \left\{ \frac{\sqrt{gh}}{2} \quad \frac{gk_x}{2} \quad \frac{gk_y}{2} \right\}^T \quad (3.99)$$

$$\lambda_3 = uk_x + vk_y - \sqrt{gh} \quad e_3 = \left\{ -\frac{\sqrt{gh}}{2} \quad \frac{gk_x}{2} \quad \frac{gk_y}{2} \right\}^T \quad (3.100)$$

Now, we define

$$L = \begin{bmatrix} 0 & \frac{\sqrt{gh}}{2} & -\frac{\sqrt{gh}}{2} \\ k_y & \frac{gk_x}{2} & \frac{gk_x}{2} \\ -k_x & \frac{gk_y}{2} & \frac{gk_y}{2} \end{bmatrix} \quad (3.101)$$

Thus

$$L^{-1} = \begin{bmatrix} 0 & k_y & -k_x \\ \frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \\ -\frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \end{bmatrix} \quad (3.102)$$

Let

$$\partial W = L^{-1} \partial E = \begin{bmatrix} 0 & k_y & -k_x \\ \frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \\ -\frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \end{bmatrix} \begin{Bmatrix} \partial H \\ \partial u \\ \partial v \end{Bmatrix} \quad (3.103)$$

and multiply both sides of Eq. (3.95) by L^{-1} . Thus, we obtain

$$L^{-1} \frac{\partial E}{\partial t} + L^{-1} A_x L L^{-1} \frac{\partial E}{\partial x} + L^{-1} A_y L L^{-1} \frac{\partial E}{\partial y} = L^{-1} R I \quad (3.104)$$

or

$$\frac{\partial W}{\partial t} + L^{-1} A_x L \frac{\partial W}{\partial x} + L^{-1} A_y L \frac{\partial W}{\partial y} = L^{-1} R I \quad (3.105)$$

or

$$\frac{\partial W}{\partial t} + \begin{bmatrix} u & \frac{gck_y}{2} & -\frac{gck_y}{2} \\ \frac{hk_y}{c} & u+ck_x & 0 \\ -\frac{hk_y}{c} & 0 & u-ck_x \end{bmatrix} \frac{\partial W}{\partial x} + \begin{bmatrix} v & -\frac{gck_x}{2} & \frac{gck_x}{2} \\ -\frac{hk_x}{c} & v+ck_y & 0 \\ \frac{hk_x}{c} & 0 & v-ck_y \end{bmatrix} \frac{\partial W}{\partial y} = L^{-1} R I \quad (3.106)$$

where

$$c = \sqrt{gh} \quad (3.107)$$

After arrangement, Eq. (3.106) can be rewritten as follows.

$$\begin{aligned} \frac{\partial W}{\partial t} + \begin{bmatrix} u & 0 & 0 \\ 0 & u+ck_x & 0 \\ 0 & 0 & u-ck_x \end{bmatrix} \frac{\partial W}{\partial x} + \begin{bmatrix} v & 0 & 0 \\ 0 & v+ck_y & 0 \\ 0 & 0 & v-ck_y \end{bmatrix} \frac{\partial W}{\partial y} \\ + \left\{ \begin{aligned} & g \left(k_y \frac{\partial H}{\partial x} - k_x \frac{\partial H}{\partial y} \right) \\ & \frac{h}{c} \left[k_y k_y \frac{\partial u}{\partial x} + k_x k_x \frac{\partial v}{\partial y} - k_x k_y \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \\ & -\frac{h}{c} \left[k_y k_y \frac{\partial u}{\partial x} + k_x k_x \frac{\partial v}{\partial y} - k_x k_y \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \end{aligned} \right\} = L^{-1} R I \end{aligned} \quad (3.108)$$

For a general consideration, we define a new L^{-1} which plays the following transformation.

$$\partial W = L^{-1} \partial E = \begin{bmatrix} 0 & k_y^{(1)} & -k_x^{(1)} \\ \frac{1}{c} & \frac{k_x^{(2)}}{g} & \frac{k_y^{(2)}}{g} \\ -\frac{1}{c} & \frac{k_x^{(2)}}{g} & \frac{k_y^{(2)}}{g} \end{bmatrix} \begin{Bmatrix} \partial H \\ \partial u \\ \partial v \end{Bmatrix} \quad (3.109)$$

Multiplying both side of Eq. (3.95) by this new L^{-1} and repeating mathematical manipulations involved in Eqs. (3.106) and (3.108) yields

$$\begin{aligned} \frac{\partial W}{\partial t} + \begin{bmatrix} u & 0 & 0 \\ 0 & u + ck_x^{(2)} & 0 \\ 0 & 0 & u - ck_x^{(2)} \end{bmatrix} \frac{\partial W}{\partial x} + \begin{bmatrix} v & 0 & 0 \\ 0 & v + ck_y^{(2)} & 0 \\ 0 & 0 & v - ck_y^{(2)} \end{bmatrix} \frac{\partial W}{\partial y} \\ + \left\{ \begin{aligned} & g \left(k_y^{(1)} \frac{\partial H}{\partial x} - k_x^{(1)} \frac{\partial H}{\partial y} \right) \\ & + \frac{h}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \\ & - \frac{h}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \end{aligned} \right\} = L^{-1} RI \end{aligned} \quad (3.110)$$

or

$$\begin{Bmatrix} \frac{DW_1}{Dt} \\ \frac{DW_2}{Dt} \\ \frac{DW_3}{Dt} \end{Bmatrix} + \begin{Bmatrix} S_1 \\ S_2 \\ S_3 \end{Bmatrix} = \begin{Bmatrix} k_y^{(1)} RI_2 - k_x^{(1)} RI_3 \\ \frac{1}{c} RI_1 + \frac{k_x^{(2)}}{g} RI_2 + \frac{k_y^{(2)}}{g} RI_3 \\ -\frac{1}{c} RI_1 + \frac{k_x^{(2)}}{g} RI_2 + \frac{k_y^{(2)}}{g} RI_3 \end{Bmatrix} \quad (3.111)$$

where

$$\frac{DW_1}{Dt} = \frac{\partial W_1}{\partial t} + u \frac{\partial W_1}{\partial x} + v \frac{\partial W_1}{\partial y} \quad (3.112)$$

$$\frac{DW_2}{Dt} = \frac{\partial W_2}{\partial t} + (u + ck_x^{(2)}) \frac{\partial W_2}{\partial x} + (v + ck_y^{(2)}) \frac{\partial W_2}{\partial y} \quad (3.113)$$

$$\frac{DW_3}{Dt} = \frac{\partial W_3}{\partial t} + (u - ck_x^{(2)}) \frac{\partial W_3}{\partial x} + (v - ck_y^{(2)}) \frac{\partial W_3}{\partial y} \quad (3.114)$$

$$S_1 = g \left(k_y^{(1)} \frac{\partial H}{\partial x} - k_x^{(1)} \frac{\partial H}{\partial y} \right) \quad (3.115)$$

$$S_2 = \frac{h}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \quad (3.116)$$

$$S_3 = \frac{-h}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \quad (3.117)$$

Note: Diagonalization can be achieved under special selections of $k_x^{(1)}$, $k_y^{(1)}$, $k_x^{(2)}$, and $k_y^{(2)}$ to make zeros of S_1 , S_2 , and S_3 .

Eq. (3.107) can be discretized, in time, as follows.

$$k_y^{(1)} \frac{u^{n+1} - u_1^*}{\Delta \tau_1} - k_x^{(1)} \frac{v^{n+1} - v_1^*}{\Delta \tau_1} + S_1 = k_y^{(1)} R I_2 - k_x^{(1)} R I_3 \quad (3.118)$$

$$\frac{1}{c} \frac{H^{n+1} - H_2^*}{\Delta \tau_2} + \frac{k_x^{(2)}}{g} \frac{u^{n+1} - u_2^*}{\Delta \tau_2} + \frac{k_y^{(2)}}{g} \frac{v^{n+1} - v_2^*}{\Delta \tau_2} + S_2 = \frac{1}{c} R I_1 + \frac{k_x^{(2)}}{g} R I_2 + \frac{k_y^{(2)}}{g} R I_3 \quad (3.119)$$

$$\frac{-1}{c} \frac{H^{n+1} - H_3^*}{\Delta \tau_3} + \frac{k_x^{(2)}}{g} \frac{u^{n+1} - u_3^*}{\Delta \tau_3} + \frac{k_y^{(2)}}{g} \frac{v^{n+1} - v_3^*}{\Delta \tau_3} + S_3 = \frac{-1}{c} R I_1 + \frac{k_x^{(2)}}{g} R I_2 + \frac{k_y^{(2)}}{g} R I_3 \quad (3.120)$$

where u_1^* , v_1^* , and $\Delta \tau_1$ are determined by backward tracking along the first characteristic; H_2^* , u_2^* , v_2^* , and $\Delta \tau_2$ are determined by backward tracking along the second characteristic; H_3^* , u_3^* , v_3^* , and $\Delta \tau_3$ are determined by backward tracking along the third characteristic; and

$$u_1^* = a_1 u_{k1}^{n+1} + a_2 u_{k2}^{n+1} + a_3 u_{k3}^{n+1} + a_4 u_{k4}^{n+1} + a_6 \quad (3.121)$$

$$v_1^* = a_1 v_{k1}^{n+1} + a_2 v_{k2}^{n+1} + a_3 v_{k3}^{n+1} + a_4 v_{k4}^{n+1} + a_7 \quad (3.122)$$

$$H_2^* = b_1 H_{j1}^{n+1} + b_2 H_{j2}^{n+1} + b_3 H_{j3}^{n+1} + b_4 H_{j4}^{n+1} + b_5 \quad (3.123)$$

$$u_2^* = b_1 u_{j1}^{n+1} + b_2 u_{j2}^{n+1} + b_3 u_{j3}^{n+1} + b_4 u_{j4}^{n+1} + b_6 \quad (3.124)$$

$$v_2^* = b_1 v_{j1}^{n+1} + b_2 v_{j2}^{n+1} + b_3 v_{j3}^{n+1} + b_4 v_{j4}^{n+1} + b_7 \quad (3.125)$$

$$H_3^* = d_1 H_{m1}^{n+1} + d_2 H_{m2}^{n+1} + d_3 H_{m3}^{n+1} + d_4 H_{m4}^{n+1} + d_5 \quad (3.126)$$

$$u_3^* = d_1 u_{m1}^{n+1} + d_2 u_{m2}^{n+1} + d_3 u_{m3}^{n+1} + d_4 u_{m4}^{n+1} + d_6 \quad (3.127)$$

$$v_3^* = d_1 v_{m1}^{n+1} + d_2 v_{m2}^{n+1} + d_3 v_{m3}^{n+1} + d_4 v_{m4}^{n+1} + d_7 \quad (3.128)$$

in which k_1, k_2, k_3 , and k_4 are nodes of the element that the backward tracking, along the first characteristic, stops in; j_1, j_2, j_3 , and j_4 are nodes of the element that the backward tracking, along the second characteristic, stops in; m_1, m_2, m_3 , and m_4 are nodes of the element that the backward tracking, along the third characteristic, stops in. (see the following figure)

- Note:* 1. $a_1 \sim a_4, b_1 \sim b_4$ and $d_1 \sim d_4$ are within the range of $[0, 1]$.
2. We may use two given parameters to determine where to stop in the backward tracking: one is for controlling tracking time and the other one is for controlling tracking distance.

Eqs. (3.118) through (3.120) can be further expressed as

$$\frac{k_y^{(1)}}{\Delta \tau_1} (u - u_1^*) - \frac{k_x^{(1)}}{\Delta \tau_1} (v - v_1^*) + \frac{k_y^{(1)}}{h} (h\kappa + SS + R - I)u - \frac{k_x^{(1)}}{h} (h\kappa + SS + R - I)v \quad (3.129)$$

$$= -g \left(k_y^{(1)} \frac{\partial H}{\partial x} - k_x^{(1)} \frac{\partial H}{\partial y} \right) + k_y^{(1)} \frac{u^T R - u^I I}{h} - k_x^{(1)} \frac{v^T R - v^I I}{h} + k_y^{(1)} \frac{\tau_x^s}{h\rho} - k_x^{(1)} \frac{\tau_y^s}{h\rho}$$

$$\begin{aligned} & \frac{1}{c \Delta \tau_2} (H - H_2^*) + \frac{k_x^{(2)}}{g \Delta \tau_2} (u - u_2^*) + \frac{k_y^{(2)}}{g \Delta \tau_2} (v - v_2^*) \\ & + \frac{k_x^{(2)}}{gh} (h\kappa + SS + R - I)u + \frac{k_y^{(2)}}{gh} (h\kappa + SS + R - I)v - \frac{u}{c} \frac{\partial Z_0}{\partial x} - \frac{v}{c} \frac{\partial Z_0}{\partial y} \end{aligned} \quad (3.130)$$

$$\begin{aligned} & = \frac{1}{c} (SS + R - I) + \frac{k_x^{(2)}}{g} \frac{u^T R - u^I I}{h} + \frac{k_y^{(2)}}{g} \frac{v^T R - v^I I}{h} \\ & + \frac{k_x^{(2)}}{g} \frac{\tau_x^s}{h\rho} + \frac{k_y^{(2)}}{g} \frac{\tau_y^s}{h\rho} - \frac{h}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \end{aligned}$$

$$\begin{aligned}
& \frac{-1}{c \Delta \tau_3} (H - H_3^*) + \frac{k_x^{(2)}}{g \Delta \tau_3} (u - u_3^*) + \frac{k_y^{(2)}}{g \Delta \tau_3} (v - v_3^*) \\
& + \frac{k_x^{(2)}}{gh} (h \kappa + SS + R - I) u + \frac{k_y^{(2)}}{gh} (h \kappa + SS + R - I) v + \frac{u}{c} \frac{\partial Z_0}{\partial x} + \frac{v}{c} \frac{\partial Z_0}{\partial y} \\
& = -\frac{1}{c} (SS + R - I) + \frac{k_x^{(2)}}{g} \frac{u^T R - u^I I}{h} + \frac{k_y^{(2)}}{g} \frac{v^T R - v^I I}{h} \\
& + \frac{k_x^{(2)}}{g} \frac{\tau_x^s}{h \rho} + \frac{k_y^{(2)}}{g} \frac{\tau_y^s}{h \rho} + \frac{h}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right]
\end{aligned} \tag{3.131}$$

In obtaining Eqs. (3.129) through (3.131), the following relationships have been employed.

$$\frac{\tau_x^b}{h \rho} = \kappa u \tag{3.132}$$

$$\frac{\tau_y^b}{h \rho} = \kappa v \tag{3.133}$$

$$F_{xx} = h \epsilon_{xx} \frac{\partial u}{\partial x} \tag{3.134}$$

$$F_{yy} = h \epsilon_{yy} \frac{\partial v}{\partial y} \tag{3.135}$$

$$F_{xy} = F_{yx} = h \epsilon_{xy} \left[\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right] \tag{3.136}$$

When u_1^* , v_1^* , H_2^* , u_2^* , v_2^* , H_3^* , u_3^* , and v_3^* are determined explicitly by using the spatial reachout option in backward tracking (i.e., track backward all the way to the previous time), Eqs. (3.129) through (3.131) can be solved node by node (H^* , u^* , v^*) as shown below.

Eqs. (3.129) through (3.131), after being multiplied by water depth (i.e., h), can be written as

$$a_{12} u + a_{13} v = b_1 \tag{3.137}$$

$$a_{21} H + a_{22} u + a_{23} v = b_2 \tag{3.138}$$

$$a_{31} H + a_{32} u + a_{33} v = b_3 \tag{3.139}$$

where

$$a_{12} = k_y^{(1)} \left[\frac{h}{\Delta \tau_1} + h \kappa + SS + R - I \right] \tag{3.140}$$

$$a_{13} = -k_x^{(1)} \left[\frac{h}{\Delta\tau_1} + h\kappa + R - I \right] \quad (3.141)$$

$$b_1 = \frac{hk_y^{(1)}}{\Delta\tau_1} u_1^* - \frac{hk_x^{(1)}}{\Delta\tau_1} v_1^* - gh \left(k_y^{(1)} \frac{\partial H}{\partial x} - k_x^{(1)} \frac{\partial H}{\partial y} \right) \\ + k_y^{(1)} (u^T R - u^I I) - k_x^{(1)} (v^T R - v^I I) + k_y^{(1)} \frac{\tau_x^s}{\rho} - k_x^{(1)} \frac{\tau_y^s}{\rho} \quad (3.142)$$

$$a_{21} = \frac{h}{c \Delta\tau_2} \quad (3.143)$$

$$a_{22} = k_x^{(2)} \left[\frac{h}{g \Delta\tau_2} + \frac{1}{g} (h\kappa + SS + R - I) \right] - \frac{h}{c} \frac{\partial Z_0}{\partial x} \quad (3.144)$$

$$a_{23} = k_y^{(2)} \left[\frac{h}{g \Delta\tau_2} + \frac{1}{g} (h\kappa + SS + R - I) \right] - \frac{h}{c} \frac{\partial Z_0}{\partial y} \quad (3.145)$$

$$b_2 = \frac{h}{c \Delta\tau_2} H_2^* + \frac{hk_x^{(2)}}{g \Delta\tau_2} u_2^* + \frac{hk_y^{(2)}}{g \Delta\tau_2} v_2^* + \frac{h}{c} (SS + R - I) + \frac{k_x^{(2)}}{g} (u^T R - u^I I) + \frac{k_y^{(2)}}{g} (v^T R - v^I I) \\ + \frac{k_x^{(2)}}{g} \frac{\tau_x^s}{\rho} + \frac{k_y^{(2)}}{g} \frac{\tau_y^s}{\rho} - \frac{h^2}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \quad (3.146)$$

$$a_{31} = \frac{-h}{c \Delta\tau_3} \quad (3.147)$$

$$a_{32} = k_x^{(2)} \left[\frac{h}{g \Delta\tau_3} + \frac{1}{g} (h\kappa + SS + R - I) \right] + \frac{h}{c} \frac{\partial Z_0}{\partial x} \quad (3.148)$$

$$a_{33} = k_y^{(2)} \left[\frac{h}{g \Delta\tau_3} + \frac{1}{g} (h\kappa + SS + R - I) \right] + \frac{h}{c} \frac{\partial Z_0}{\partial y} \quad (3.149)$$

$$b_3 = \frac{-h}{c \Delta\tau_3} H_3^* + \frac{hk_x^{(2)}}{g \Delta\tau_3} u_3^* + \frac{hk_y^{(2)}}{g \Delta\tau_3} v_3^* - \frac{h}{c} (SS + R - I) + \frac{k_x^{(2)}}{g} (u^T R - u^I I) + \frac{k_y^{(2)}}{g} (v^T R - v^I I) \\ + \frac{k_x^{(2)}}{g} \frac{\tau_x^s}{\rho} + \frac{k_y^{(2)}}{g} \frac{\tau_y^s}{\rho} + \frac{h^2}{c} \left[k_y^{(2)} k_y^{(2)} \frac{\partial u}{\partial x} + k_x^{(2)} k_x^{(2)} \frac{\partial v}{\partial y} - k_x^{(2)} k_y^{(2)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \quad (3.150)$$

Therefore, we solve Eqs. (3.137) through (3.139) for H^* , u^* , v^* arithmetically. Now, we can solve

Eq. (3.94) as follows. Eq. (3.94) can be written in details as

$$\frac{H - H^{\#}}{\Delta t} = 0 \quad (3.151)$$

$$\frac{h(u - u^{\#})}{\Delta t} = \left[\frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y} \right] \quad (3.152)$$

$$\frac{h(v - v^{\#})}{\Delta t} = \left[\frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y} \right] \quad (3.153)$$

Eq. (3.151) gives that $H = H^{\#}$, while Eqs. (3.152) and (3.153) can be discretized, in the finite element method, as

$$\frac{h}{\Delta t} [QA] \{u\} + [QD^1] \{u\} + [QD^4] \{v\} = \{QR^1\} + \{BQ^1\} \quad (3.154)$$

$$\frac{h}{\Delta t} [QA] \{v\} + [QD^2] \{u\} + [QD^3] \{v\} = \{QR^2\} + \{BQ^2\} \quad (3.155)$$

where

$$QA_{ij} = \sum_{e \in M_e} \int_{R_e} N_{\alpha}^e N_{\beta}^e dR \quad (3.156)$$

$$QD_{ij}^1 = \sum_{e \in M_e} \int_{R_e} \nabla N_{\alpha}^e \cdot \begin{bmatrix} h\epsilon_{xx} & 0 \\ 0 & h\epsilon_{xy} \end{bmatrix} \cdot \nabla N_{\beta}^e dR \quad (3.157)$$

$$QD_{ij}^2 = \sum_{e \in M_e} \int_{R_e} \nabla N_{\alpha}^e \cdot \begin{bmatrix} 0 & h\epsilon_{xy} \\ 0 & 0 \end{bmatrix} \cdot \nabla N_{\beta}^e dR \quad (3.158)$$

$$QD_{ij}^3 = \sum_{e \in M_e} \int_{R_e} \nabla N_{\alpha}^e \cdot \begin{bmatrix} h\epsilon_{xy} & 0 \\ 0 & h\epsilon_{yy} \end{bmatrix} \cdot \nabla N_{\beta}^e dR \quad (3.159)$$

$$QD_{ij}^4 = \sum_{e \in M_e} \int_{R_e} \nabla N_{\alpha}^e \cdot \begin{bmatrix} 0 & 0 \\ h\epsilon_{xy} & 0 \end{bmatrix} \cdot \nabla N_{\beta}^e dR \quad (3.160)$$

$$QR_i^1 = \sum_{e \in M_e} \int_{R_e} N_{\alpha}^e \frac{hu^{\#}}{\Delta t} dR \quad (3.161)$$

$$QR_i^2 = \sum_{e \in M_c} \int_{R_e} N_\alpha^e \frac{h v^*}{\Delta t} dR \quad (3.162)$$

$$BQ_i^1 = \sum_{e \in M_c} \int_{B_e} \left\{ N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} h\epsilon_{xx} & 0 \\ 0 & h\epsilon_{xy} \end{bmatrix} \cdot \nabla u + N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} 0 & 0 \\ h\epsilon_{xy} & 0 \end{bmatrix} \cdot \nabla v \right\} dB \quad (3.163)$$

$$BQ_i^2 = \sum_{e \in M_c} \int_{B_e} \left\{ N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} 0 & h\epsilon_{xy} \\ 0 & 0 \end{bmatrix} \cdot \nabla u + N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} h\epsilon_{xy} & 0 \\ 0 & h\epsilon_{yy} \end{bmatrix} \cdot \nabla v \right\} dB \quad (3.164)$$

In solving Eqs. (3.129) through (3.131) at boundary nodes, we demonstrate how boundary conditions are implemented as in the following. An overland boundary segment can be either a closed or an open (flow-through) boundary. In the former case, nothing needs to be specified. While in the latter case, H , u , and v of the approaching flow, with respect to the characteristic ongoing direction, must be given at all segments (or segment nodes). Some details are given for both cases.

< Case 1 > Closed boundaries

:

The first characteristic equation is always replaced by the following equation, representing a zero normal flux on the boundary.

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad (3.165)$$

where \mathbf{n} is the outward unit normal vector of the boundary segment. Tracking along the closed boundary will be used for the second and third characteristics if necessary.

< Case 2 > Open boundaries:

The first characteristic equation is always replaced by the following equation, representing a zero lateral flux on the boundary.

$$\mathbf{n}_\perp \cdot \mathbf{u} = 0 \quad (3.166)$$

where \mathbf{n}_\perp is the unit vector parallel to the segment. Either the second or the third characteristic equation, depending on the propagation direction, will be replaced by the boundary condition specified on the boundary. There are four types of boundary conditions considered here. Only when the propagation direction is inward to the domain of interest, will the replacement be employed.

(1) Given time-dependent normal flux, $q(t)$: (used for upstream open boundaries)

$$\mathbf{n} \cdot \mathbf{u} = \frac{q}{h} \quad (3.167)$$

(2) Given time-dependent water stage, $H(t)$: (used for either upstream or downstream boundaries)

$$H = H_b \quad (3.168)$$

(3) Given water depth-dependent normal flux, $q(h)$: (used for natural downstream open boundaries)

or river/stream-/junction-related boundaries)

$$\mathbf{n} \cdot \mathbf{u} = \frac{q}{h} \quad (3.169)$$

(4) Given stage difference-dependent normal flux, $q(\Delta H)$: (used for river/stream-/junction-related boundaries)

$$\mathbf{n} \cdot \mathbf{u} = \frac{q_n}{h} \quad (3.170)$$

As mentioned earlier in Section 3.1.2, both depth and velocity must be specified on the boundary where supercritical flow occurs.

3.2.2. The Lagrangian approach for both 2-D diffusion and 2-D kinematic wave models

Recall Eqs. (2.9), (2.12), and (2.13)

$$\frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} + \frac{\partial hv}{\partial y} = SS + R - I \quad (3.171)$$

where

$$u = \frac{-1}{n} \left[\frac{h}{1 + (\nabla Z_0)^2} \right]^{2/3} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \quad (3.172)$$

$$v = \frac{-1}{n} \left[\frac{h}{1 + (\nabla Z_0)^2} \right]^{2/3} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial y} \quad (3.173)$$

Substituting Eqs. (3.168) and (3.169) into Eq. (3.167) yields

$$\frac{\partial h}{\partial t} + \frac{5u}{3} \frac{\partial h}{\partial x} + \frac{5v}{3} \frac{\partial h}{\partial y} = SS + R - I - X - Y \quad (3.174)$$

where

$$\begin{aligned} X = & \frac{-1}{n} \frac{h^{5/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial^2(Z_0 + h)}{\partial x^2} + \frac{1}{n^2} \frac{h^{5/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \frac{\partial n}{\partial x} \\ & + \frac{-2}{n} \frac{h^{5/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{\partial(Z_0 + h)}{\partial x} \frac{-1}{4} \left[\left(\frac{\partial(Z_0 + h)}{\partial x} \right)^2 + \left(\frac{\partial(Z_0 + h)}{\partial y} \right)^2 \right]^{-5/4} \\ & \left[\frac{\partial(Z_0 + h)}{\partial x} \frac{\partial^2(Z_0 + h)}{\partial x^2} + \frac{\partial(Z_0 + h)}{\partial y} \frac{\partial^2(Z_0 + h)}{\partial x \partial y} \right] \\ & + \frac{-2}{n} \frac{h^{5/3}}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial x} \frac{-2}{3} [1 + (\nabla Z_0)^2]^{-5/3} \left[\frac{\partial Z_0}{\partial x} \frac{\partial^2 Z_0}{\partial x^2} + \frac{\partial Z_0}{\partial y} \frac{\partial^2 Z_0}{\partial x \partial y} \right] \end{aligned} \quad (3.175)$$

$$\begin{aligned}
Y = & \frac{-1}{n} \frac{h^{5/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial^2(Z_0 + h)}{\partial y^2} + \frac{1}{n^2} \frac{h^{5/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{1}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial y} \frac{\partial n}{\partial y} \\
& + \frac{-2}{n} \frac{h^{5/3}}{[1 + (\nabla Z_0)^2]^{2/3}} \frac{\partial(Z_0 + h)}{\partial y} \frac{-1}{4} \left[\left(\frac{\partial(Z_0 + h)}{\partial x} \right)^2 + \left(\frac{\partial(Z_0 + h)}{\partial y} \right)^2 \right]^{-5/4} \\
& \left[\frac{\partial(Z_0 + h)}{\partial x} \frac{\partial^2(Z_0 + h)}{\partial x \partial y} + \frac{\partial(Z_0 + h)}{\partial y} \frac{\partial^2(Z_0 + h)}{\partial y^2} \right] \\
& + \frac{-2}{n} \frac{h^{5/3}}{[\nabla(Z_0 + h)]^{1/2}} \frac{\partial(Z_0 + h)}{\partial y} \frac{-2}{3} [1 + (\nabla Z_0)^2]^{5/3} \left[\frac{\partial Z_0}{\partial x} \frac{\partial^2 Z_0}{\partial x \partial y} + \frac{\partial Z_0}{\partial y} \frac{\partial^2 Z_0}{\partial y^2} \right]
\end{aligned} \tag{3.176}$$

Eq. (3.174) can be further written as

$$\frac{Dh}{Dt} = SS + R - I - X - Y \tag{3.177}$$

where the following characteristic equations apply.

$$\frac{dx}{dt} = \frac{5}{3} u \tag{3.178}$$

$$\frac{dy}{dt} = \frac{5}{3} v \tag{3.179}$$

Hence the solution to Eq. (3.177) is

$$h(x, y, t) = h(x_0, y_0, 0) + (R - I - X - Y)t \tag{3.180}$$

in which

$$x - x_0 = \int_0^t \frac{5}{3} u dt \tag{3.181}$$

$$y - y_0 = \int_0^t \frac{5}{3} v dt \tag{3.182}$$

A nonlinear iteration loop with the Picard method implemented is used to solve Eqs. (3.78) through (3.80) in the dynamic wave model or to solve Eqs. (3.171) through (3.173) in the diffusion wave model during each time step.

3.3. Solving the 3-D subsurface flow equations

The Richard's equation is discretized with the Galerkin finite element method in space and with the finite difference method in time. In the model, the steady-state version of subsurface flow equations can be

solved for determining the initial subsurface flow condition when boundary conditions are complicated and/or unsaturated zones are taken into account. The details of solving the Richard's equation has been described elsewhere [Yeh et al,] and are not to be presented here.

To adequately handle the flow through surface/subsurface interface, the following points have been implemented in the computer code.

(1) If the flow direction is determined from subsurface to surface, seepage occurs when the pressure head at the corresponding subsurface node is positive; otherwise, evaporation happens.

(2) When rainfall is negative, it appears as a sink to the surface system when the overland is wet (i.e., water depth is greater than zero); otherwise, it is a sink to the subsurface system.

3.4. Solving the 1-D river/stream transport equations

In solving the transport equations of both 1-D river/stream and 2-D overland, the following strategy is employed.

<Strategy> Using the predictor-corrector scheme to deal with transport equations of mobile materials.

In solving Eqs. (2.23), (2.25), and (2.26), the following strategy is employed. All the three equations can be expressed in the following form.

$$A \frac{dC}{dt} = L(C) + \text{RHS} \quad (3.183)$$

where C can be S_n , C_i^w , or $S_n C_{ni}^s$, L is the diffusion operator, and RHS represents source/sink terms.

Thus, we can solve Eq. (3.183) with the following two steps.
First, we solve

$$A \frac{C^{N+1/2} - C^N}{\Delta \tau} = L(C^{N+1/2}) + (\text{RHS})^N \quad (3.184)$$

Second, we solve

$$A \frac{C^{N+1} - C^N}{\Delta \tau} = L(C^{N+1/2}) + (\text{RHS})^{N+1} \quad (3.185)$$

We can also subtract Eq. (3.184) from Eq. (3.185) to yield

$$A \frac{C^{N+1} - C^{N+1/2}}{\Delta \tau} = (\text{RHS})^{N+1} - (\text{RHS})^N \quad (3.186)$$

The advantage of solving Eq. (3.186), rather than Eq. (3.185), is that we can compute C^{N+1} node by node when $C^{N+1/2}$ is previously determined. Thus, we first solve Eq. (3.184) for $C^{N+1/2}$ (the intermediate value) in the so-called predictor step and perform the so-called corrector step by solving Eq. (3.186) to obtain C^{N+1} . To avoid negative numerical results in solving Eq. (3.184), the following equation is actually solved when $(\text{RHS})^N$ is negative.

$$A \frac{C^{N+1/2} - C^N}{\Delta \tau} - \frac{(RHS)^N}{C^N} C^{N+1/2} = L(C^{N+1/2}) \quad (3.187)$$

Consequently, we are solving the following equation in the corrector step.

$$A \frac{C^{N+1} - C^{N+1/2}}{\Delta \tau} = (RHS)^{N+1} - \frac{(RHS)^N}{C^N} C^{N+1/2} \quad (3.188)$$

With the finite element approximation, Eq. (3.184) can be discretized as follows.

$$\left(\frac{[QA]}{\Delta \tau} + w [QD] \right) \{C\} = \{QR\} + (1-w) [QD] \{C^P\} + \{QB\} \quad (3.189)$$

where the associated element matrices are defined as follows.

$$[QA]^e = \int_e N_i A N_j dx \quad (3.190)$$

$$[QD]^e = \int_e \frac{dN_i}{dx} A K_x \frac{dN_j}{dx} dx \quad (3.191)$$

$$\{QR\}^e = \int_e N_i (RHS)^N dx \quad (3.192)$$

$$\{QB\}^e = - \left(-A K_x \frac{\partial C}{\partial x} \right)_{\text{boundary}} \quad (3.193)$$

It is noted that both $[QA]^e$ and $\{QR\}^e$ must be lumped such that Eqs. (3.184) and (3.186) are solved consistently. Also, boundary conditions for mobile materials are implemented in this predictor step.

In the following, we show the procedures of solving the transport system in Section 3.3.1, to determine the concentrations of chemicals and sediments at junctions in Section 3.3.2, and to give estimation of deposition and erosion in Section 3.3.3.

3.4.1. Procedures of solving 1-D river/stream transport equations

Recall Eqs. (2.35) through (2.39) and express them in the Lagrangian form for mobile materials as follows.

For the continuity equation of suspended sediment:

$$A \frac{dS_n}{dt} = A \frac{\partial S_n}{\partial t} + Q \frac{\partial S_n}{\partial x} = 0 \quad (3.194)$$

$$A \frac{dS_n}{dt} - \frac{\partial}{\partial x} \left[A K_x \frac{\partial S_n}{\partial x} \right] = [M_n^s + PR_n - PD_n + M_n^{os}] - [SS + R - I + R_1 + R_2] S_n \quad n \in [1, N_s] \quad (3.195)$$

For the continuity equation of bed sediment:

$$\frac{\partial M_n}{\partial t} = D_n - R_n \quad n \in [1, N_s] \quad (3.196)$$

For the continuity equation of dissolved chemical:

$$A \frac{dC_i^w}{dt} = A \frac{\partial C_i^w}{\partial t} + Q \frac{\partial C_i^w}{\partial x} = 0 \quad (3.197)$$

$$\begin{aligned} A \frac{dC_i^w}{dt} - \frac{\partial}{\partial x} \left[A K_x \frac{\partial C_i^w}{\partial x} \right] = & \left[M_i^{cw} + A k_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n A C_{ni}^s + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n P C_{ni}^b + M_i^{crw} - M_i^{ciw} + M_i^{cow} \right] \\ & + \sum_{m=1}^{N_{rx}} (a_{mj}^c - b_{mj}^c) k_m^{rb} A \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \right] \\ & - \left[\lambda_i^c A + A k_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} + SS + R - I + R_1 + R_2 \right] C_i^w \quad i \in [1, N_c] \end{aligned} \quad (3.198)$$

For the continuity equation of particulate chemical on suspended sediment:

$$A \frac{d(S_n C_{ni}^s)}{dt} = A \frac{\partial (S_n C_{ni}^s)}{\partial t} + Q \frac{\partial (S_n C_{ni}^s)}{\partial x} = 0 \quad (3.199)$$

$$\begin{aligned} A \frac{d(S_n C_{ni}^s)}{dt} - \frac{\partial}{\partial x} \left[A K_x \frac{\partial (S_n C_{ni}^s)}{\partial x} \right] = & \left[M_{ni}^{cs} + k_{ni}^{sf} S_n A C_i^w + B \frac{R_n}{M_n} (M_n C_{ni}^b) - B \frac{D_n}{S_n} (S_n C_{ni}^s) + M_{ni}^{cos} \right] \\ & - \left[\lambda_{ni}^s A + k_{ni}^{sb} A + SS + R - I + R_1 + R_2 \right] (S_n C_{ni}^s) \quad n \in [1, N_s], i \in [1, N_c] \end{aligned} \quad (3.200)$$

For the continuity equation of particulate chemical on bed sediment:

$$\begin{aligned} \frac{\partial (M_n C_{ni}^b)}{\partial t} = & \left[\frac{D_n}{S_n} (S_n C_{ni}^s) - \frac{R_n}{M_n} (M_n C_{ni}^b) + k_{ni}^{bf} M_n C_i^w \right] - \left[\lambda_{ni}^b + k_{ni}^{bb} \right] (M_n C_{ni}^b) \\ & n \in [1, N_s], i \in [1, N_c] \end{aligned} \quad (3.201)$$

We solve the transport system by achieving the following steps.

Step 1 Solve Eqs. (3.194), (3.197), and (3.199) to obtain the Lagrangian values for suspended sediments, dissolved chemicals, and particulate chemicals on suspend sediments.

Step 2 Solve Eqs. (3.195) and (3.196) for S_n and M_n .

(a) Solve Eq. (3.195) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eq. (3.195))

==> Obtaining the intermediate value for suspended sediments.

(b) Prepare the corrector form of Eqs. (3.195) as described in Eq. (3.186). It can be written as follows.

$$\begin{aligned} A \frac{(S_n)^{N+1} - (S_n)^{N+1/2}}{\delta t} \\ = (RHS_n^s)^{N+1} - (RHS_n^s)^N \quad \left(\text{if } (RHS_n^s)^N \geq 0 \right) \\ = (RHS_n^s)^{N+1} - \frac{(RHS_n^s)^N}{(S_n)^N} (S_n)^{N+1/2} \quad \left(\text{if } (RHS_n^s)^N < 0 \right) \quad n \in [1, N_s] \end{aligned} \quad (3.202)$$

where

$$(RHS_n^s) = [M_n^s + PR_n - PD_n + M_n^{os}] + [SS + R - I + R_1 + R_2] S_n \quad n \in [1, N_s] \quad (3.203)$$

(c) Solve Eq. (3.202) and Eq. (3.196) node by node with the Picard method to obtain the concentrations of suspended and bed sediments.

Note: In Eqs. (3.195) and (3.196) both D_n and R_n need to be evaluated first, while in Eq. (3.195) A , Q , K_x , P , R , I , R_1 , R_2 , M_n^s , and M_n^{os} are either given or determined after the flow equations are solved. During each iteration in (c), both Eq. (3.202) and (3.196) are solved with the time-implicit scheme.

Step 3 Solve Eqs. (3.198), (3.200), and (3.201) for C_i^w , C_{ni}^s , and C_{ni}^b .

(a) Solve Eqs. (3.198) and (3.200) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eqs. (3.198) and (3.200)).

(b) Prepare the corrector form of Eqs. (3.198) and (3.200) described in Eq. (3.186). They can be written as follows.

For dissolved chemicals:

$$\begin{aligned} A \frac{(C_i^w)^{N+1} - (C_i^w)^{N+1/2}}{\delta t} \\ = (RHS_i^c)^{N+1} - (RHS_i^c)^N \quad \left(\text{if } (RHS_i^c)^N \geq 0 \right) \\ = (RHS_i^c)^{N+1} - \frac{(RHS_i^c)^N}{(C_i^w)^N} (C_i^w)^{N+1/2} \quad \left(\text{if } (RHS_i^c)^N < 0 \right) \quad i \in [1, N_c] \end{aligned} \quad (3.204)$$

where

$$\begin{aligned}
(RHS_i^c) = & \left[M_i^{cw} + A k_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n A C_{ni}^s + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n P C_{ni}^b + M_i^{crw} - M_i^{ciw} + M_i^{cow} \right] \\
& - \left[\lambda_i^c A + A k_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} + SS + R - I + R_1 + R_2 \right] C_i^w \\
& + \sum_{m=1}^{N_n} (a_{mj}^c - b_{mj}^c) k_m^{rb} A \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \right] \quad i \in [1, N_c]
\end{aligned} \quad (3.205)$$

For particulate chemicals on suspended sediments:

$$\begin{aligned}
& A \frac{(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2}}{\delta t} \\
& = (RHS_{ni}^s)^{N+1} - (RHS_{ni}^s)^N \quad \left(\text{if } (RHS_{ni}^s)^N \geq 0 \right) \\
& = (RHS_{ni}^s)^{N+1} - \frac{(RHS_{ni}^s)^N}{(C_{ni}^s)^N} (C_{ni}^s)^{N+1/2} \quad \left(\text{if } (RHS_{ni}^s)^N < 0 \right) \quad n \in [1, N_s], i \in [1, N_c]
\end{aligned} \quad (3.206)$$

where

$$\begin{aligned}
(RHS_{ni}^s) = & \left[M_{ni}^{cs} + k_{ni}^{sf} S_n A C_i^w + B \frac{R_n}{M_n} (M_n C_{ni}^b) - B \frac{D_n}{S_n} (S_n C_{ni}^s) + M_{ni}^{cos} \right] \\
& - \left[\lambda_{ni}^s A + k_{ni}^{sb} A + SS + R - I + R_1 + R_2 \right] (S_n C_{ni}^s) \quad n \in [1, N_s], i \in [1, N_c]
\end{aligned} \quad (3.207)$$

(c) Solve Eqs. (3.204), (3.206), and (3.201) node by node with the Newton-Raphson method.

Note: In Eqs. (3.204), (3.206), and (3.201) S_n and M_n are computed in Step 1, while A , Q , B , P , K_x , reaction rate constants, stoichiometry, 1-st order decay constants, partial atmospheric pressure, and sources/sinks are either given or determined after the flow equations are solved. To achieve the (c) of Step 3, the following residual equations are constructed.

For dissolved chemicals:

$$\begin{aligned}
& (RES_i^c) \\
& = A \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t \left[(RHS_i^c)^{N+1} - (RHS_i^c)^N \right] \quad \left(\text{if } (RHS_i^c)^N \geq 0 \right) \\
& = A \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t \left[(RHS_i^c)^{N+1} - \frac{(RHS_i^c)^N}{(C_i^w)^N} (C_i^w)^{N+1/2} \right] \quad \left(\text{if } (RHS_i^c)^N < 0 \right) \\
& \quad i \in [1, N_c]
\end{aligned} \quad (3.208)$$

For particulate chemicals on suspended sediments:

$$\begin{aligned}
 (\text{RES}_{ni}^s) &= A \left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2} \right] - \delta t \left[(\text{RHS}_{ni}^s)^{N+1} - (\text{RHS}_{ni}^s)^N \right] \quad \left(\text{if } (\text{RHS}_{ni}^s)^N \geq 0 \right) \\
 &= A \left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2} \right] - \delta t \left[(\text{RHS}_{ni}^s)^{N+1} - \frac{(\text{RHS}_{ni}^s)^N}{(S_n C_{ni}^s)^N} (S_n C_{ni}^s)^{N+1/2} \right] \quad \left(\text{if } (\text{RHS}_{ni}^s)^N < 0 \right) \quad (3.209) \\
 &\quad n \in [1, N_s], \quad i \in [1, N_c]
 \end{aligned}$$

For particulate chemicals on bed sediments:

$$(\text{RES}_{ni}^b) = (M_n C_{ni}^b)^{N+1} - (M_n C_{ni}^b)^N - \Delta t (\text{RHS}_{ni}^b)^{N+1} \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.210)$$

The associated Jacobian entries are thus computed as shown in the following.

For dissolved chemicals:

$$\begin{aligned}
 \frac{\partial (\text{RES}_i^c)}{\partial (C_1^w)^{N+1}} &= \delta_{il} A + \delta_{il} \delta t \left[\lambda_i^c A + SS + R - I + R_1 + R_2 + A k_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} \right] - \\
 &\quad \delta t \left[\sum_{m=1}^{N_\alpha} (a_{mi}^c - b_{mi}^c) A \left(k_m^{rb} b_{mi}^c (C_1^w)^{b_{mi}^c - 1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{b_{mj}^c} - k_m^{rf} a_{mi}^c (C_1^w)^{a_{mi}^c - 1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{a_{mj}^c} \right) \right] \quad (3.211) \\
 &\quad i \in [1, N_c]
 \end{aligned}$$

$$\frac{\partial (\text{RES}_i^c)}{\partial (S_n C_{ni}^s)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sb} A \quad n \in [1, N_s], \quad i \in [1, N_c], \quad (3.212)$$

$$\frac{\partial (\text{RES}_i^c)}{\partial (M_n C_{ni}^b)^{N+1}} = -\delta_{il} \delta t k_{ni}^{bb} P \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.213)$$

For particulate chemicals on suspended sediments:

$$\frac{\partial (\text{RES}_{ni}^s)}{\partial (C_1^w)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sf} S_n A \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.214)$$

$$\begin{aligned}
 \frac{\partial (\text{RES}_{ni}^s)}{\partial (S_n C_{ni}^s)^{N+1}} &= \delta_{il} A + \delta_{il} \delta t B \frac{D_n}{S_n} + \delta_{il} \delta t \left[\lambda_{ni}^s A + k_{ni}^{sb} A + SS + R - I + R_1 + R_2 \right] \\
 &\quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.215)
 \end{aligned}$$

$$\frac{\partial(\text{RES}_{ni}^s)}{\partial(M_n C_{nl}^b)^{N+1}} = -\delta_{il} \delta t B \frac{R_n}{M_n} \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.216)$$

For particulate chemicals on bed sediments:

$$\frac{\partial(\text{RES}_{ni}^b)}{\partial(C_1^w)^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bf} M_n \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.217)$$

$$\frac{\partial(\text{RES}_{ni}^b)}{\partial(S_n C_{nl}^s)^{N+1}} = -\delta_{il} \Delta t \frac{D_n}{S_n} \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.218)$$

$$\frac{\partial(\text{RES}_{ni}^b)}{\partial(M_n C_{nl}^b)^{N+1}} = \delta_{il} + \delta_{il} \Delta t \frac{R_n}{M_n} + \delta_{il} \Delta t [\lambda_{ni}^b + k_{ni}^{bb}] \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.219)$$

It is noted that if SS, R, R1, and R2 are negative (i.e., sinks), they should not appear in Eqs. (3.211) and (3.215). Likewise, if I is positive (i.e., sink), it must not appear in the two equations.

3.4.2. Determining chemical and sediment concentrations at junctions

At junctions, the following equations are employed to determine the concentrations of chemicals and sediments.

For suspended sediment:

$$\frac{dV(j)S_n(j)}{dt} = \sum_{k=1}^{N_{JTH}(j)} Q^k S_n^k + M_n^s(j) + M_n^{os}(j) + [R_n(j) - D_n(j)] AJT(j) \quad n \in [1, N_s] \quad (3.220)$$

For bed sediment:

$$\frac{\partial M_n(j)}{\partial t} = D_n(j) - R_n(j) \quad n \in [1, N_s] \quad (3.221)$$

For dissolved chemical:

$$\begin{aligned}
& \frac{dV(j)C_i^w(j)}{dt} \\
&= \sum_{k=1}^{N_{JTH}(j)} Q^k C_i^{wk} + M_i^{cw}(j) - \lambda_i^c V(j) C_i^w(j) + M_i^{crw}(j) - M_i^{ciw}(j) + M_i^{cow}(j) \\
&+ V(j) k_i^{ab} \left[p_i - \frac{k_i^{af}}{k_i^{ab}} C_i^w(j) \right] + \sum_{n=1}^{N_s} k_{ni}^{sb} V(j) \left[(S_n(j) C_{ni}^s(j)) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} S_n(j) C_i^w(j) \right] \\
&+ \sum_{n=1}^{N_s} k_{ni}^{bb} AJT(j) \left[(M_n(j) C_{ni}^b(j)) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} M_n(j) C_i^w(j) \right] \\
&+ \sum_{m=1}^{N_{rx}} (a_{mi}^c - b_{mi}^c) k_m^{rb} V(j) \left[\prod_{j=1}^{N_c} (C_j^w(j))^{b_{mj}^c} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w(j))^{a_{mj}^c} \right] \quad i \in [1, N_c]
\end{aligned} \tag{3.222}$$

For particulate chemical on suspended sediment:

$$\begin{aligned}
& \frac{dV(j)(S_n(j)C_{ni}^s(j))}{dt} \\
&= \sum_{k=1}^{N_{JTH}(j)} Q^k (S_n C_{ni}^{sk}) + M_{ni}^{cs}(j) - \lambda_{ni}^s V(j) (S_n(j) C_{ni}^s(j)) - \frac{D_n(j)}{S_n(j)} AJT(j) (S_n(j) C_{ni}^s(j)) \\
&- k_{ni}^{sb} V(j) \left[(S_n(j) C_{ni}^s(j)) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} S_n(j) C_i^w(j) \right] + \frac{R_n(j)}{M_n(j)} AJT(j) (M_n(j) C_{ni}^b(j)) + M_{ni}^{cos}(j) \\
&n \in [1, N_s], i \in [1, N_c]
\end{aligned} \tag{3.223}$$

For particulate chemical on bed sediment:

$$\begin{aligned}
& \frac{\partial (M_n(j) C_{ni}^b(j))}{\partial t} \\
&= \frac{D_n(j)}{S_n(j)} (S_n(j) C_{ni}^s(j)) - \frac{R_n(j)}{M_n(j)} (M_n(j) C_{ni}^b(j)) - \lambda_{ni}^b(j) M_n(j) C_{ni}^b(j) \\
&- k_{ni}^{bb} \left[(M_n(j) C_{ni}^b(j)) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} M_n(j) C_i^w(j) \right] \quad n \in [1, N_s], i \in [1, N_c]
\end{aligned} \tag{3.224}$$

where

- $V(j)$ = The volume of water at the j-th junction [L^3];
- $AJT(j)$ = The horizontal area of the j-th junction [L^2].
- $D_n(j)$ = Deposition rate of the n-th size fraction sediment at the j-th junction [$M/L^2/T$];

$R_n(j)$	=	Erosion rate of the n-th size fraction sediment $[M/L^2/T]$;
$S_n(j)$	=	Volumetrically averaged sediment concentration of the n-th fraction size at the j-th junction $[M/L^3]$;
$M_n(j)$	=	Sediment mass per unit bed area of the n-th size fraction at the j-th junction at the j-th junction $[M/L^2]$;
$NJ_{RTH}(j)$	=	Number of river/stream reaches which connect to the j-th junction;
Q^k	=	The flow rate from the k-th connected river/stream reach to the junction $[L^3/T]$, it is positive if coming in and negative if going out;
S_n^k	=	The concentration of the n-th sized suspended sediment from the k-th connected river/stream reach to the junction $[M/L^3]$;
C_i^{wk}	=	The concentration of the i-th dissolved chemical from the k-th connected river/stream reach to the junction $[M/L^3]$;
C_{ni}^{sk}	=	The concentration of the i-th particulate chemical on the n-th sized suspended sediment from the k-th connected river/stream reach to the junction $[M/L^3]$;
$M_n^s(j)$	=	Source of the n-th suspended sediment at the j-th junction $[M/T]$;
$M_n^{os}(j)$	=	Source of the n-th suspended sediment from overland flow to the j-th junction $[M/T]$;
$C_i^w(j)$	=	Volometrically-averaged concentration of the i-th dissolved chemical at the j-th junction $[M/L^3]$;
$C_{ni}^b(j)$	=	Volometrically-averaged particulate chemical concentration on bed sediment of the n-th fraction size at the j-th junction $[M/M]$;
$C_{ni}^s(j)$	=	Volometrically-averaged particulate chemical concentration on suspended sediment of the n-th fraction size at the j-th junction $[M/M]$;
$M_{ni}^{cs}(j)$	=	Source of the i-th particulate chemical on suspended sediment of the n-th fraction size at the j-th junction $[M/T]$;
$M_{ni}^{cos}(j)$	=	Source of the i-th particulate chemical on suspended sediment of the n-th fraction size from overland to the j-th junction $[M/T]$;
$M_i^{cw}(j)$	=	Source of the i-th dissolved chemical at the j-th junction $[M/T]$;
$M_i^{crw}(j)$	=	Rainfall source of the i-th dissolved chemical at the j-th junction $[M/T]$;
$M_i^{ciw}(j)$	=	Infiltration sink of the i-th dissolved chemical at the j-th junction $[M/T]$;
$M_i^{cow}(j)$	=	Source of the i-th dissolved chemical from overland to the j-th junction $[M/T]$.

Eqs. (3.220) and (3.221) are solved first by using the Picard method, while Eqs. (3.222) through (3.224) are solved with the Newton-Raphson method.

3.4.3. Estimation of Deposition and Erosion

We estimate the deposition and erosion rates by using the following equations.

< Case 1 > Cohesive sediments: (e.g., silt and clay)

$$D_n = V_{sn} S_n \left[1 - \frac{\tau_b}{\tau_{cDn}} \right] \quad (3.225)$$

$$R_n = E_n \left[\frac{\tau_b}{\tau_{cRn}} - 1 \right] \quad (3.226)$$

where V_{sn} is the settling velocity of the n-th size fraction sediment $[L/T]$; τ_b is the bottom shear stress or the

bottom friction stress $[M/L/T^2]$; τ_{cDn} is the critical shear stress for the deposition of the n-th size fraction sediment $[M/L/T^2]$; τ_{cRn} is the critical shear stress for the erosion of the n-th size fraction sediment $[M/L/T^2]$; E_n is the erodibility of the n-th size fraction sediment $[M/L^2]$. In the computer code, V_{sn} , τ_{cDn} , τ_{cRn} , and E_n are input parameters, while τ_b is computed in the flow module.

< Case 2 > Non-cohesive sediments: (e.g., sand)

$$D_n = \frac{G_{sAn} - G_{sn}}{\Delta L} \quad (3.227)$$

$$R_n = \frac{G_{sn} - G_{sAn}}{\Delta L} \quad (3.228)$$

where G_{sAn} is the actual load rate of the n-th size fraction sediment per unit width at a upstream location $[M/L/T]$; G_{sn} is the maximum load rate (capacity) of the n-th size fraction sediment per unit width at a downstream location $[M/L/T]$; ΔL is the distance between the upstream and the downstream locations. In the computer code, ΔL can be determined based on the coordinates, while G_{sAn} and G_{sn} are computed based on the following equations.

$$G_{sAn} = S_n * u * r \quad (3.229)$$

$$G_{sn} = 10 \frac{\rho^2 u r S (\tau_b - \tau_{cm})}{g d_n (\rho_{sn} - \rho)^2} \quad (3.230)$$

where ρ is the fluid density $[M/L^3]$; ρ_{sn} is the density of the n-th size fraction sediment $[M/L^3]$; u is river/stream flow velocity $[L/T]$; r is hydraulic radius $[L]$; S the friction slope, d_n is the median diameter of the n-th size fraction sediment particle $[L]$; g is gravity $[L/T^2]$; τ_{cm} is the critical bottom shear stress of the n-th size fraction sediment at which sediment movement begins $[M/L/T^2]$. Among these parameters, ρ , ρ_{sn} , d_n , and τ_{cm} are input by users, while u , r , and S are estimated in the flow module.

Note: Eq. (3.230) is from "Hydraulics of Sediment Transport" by Walter Hans Graf (1984), Water Resources Publication, Eq. (7.14) on page 128. Eqs. (3.225) through (3.228) can be found from "CHNTRN: A Channel Transport Model for Simulating Sediment and Chemical Distribution in a Stream/River Network" by Yeh (1983), ORNL-5882 Report, Eqs. (29) and (30) on page 12.

3.5. Solving the 2-D overland transport equations

The strategy for solving 2-D overland transport equations has been described in the previous section and will not be repeated here. In the following, we are to go through the procedures of solving the 2-D transport system, like what we have achieved in Section 3.3.1 for 1-D river/stream transport. Recall Eqs. (2.53) through (2.57) and express them in the Lagrangian form for mobile materials as follows.

For the continuity equation of suspended sediment:

$$h \frac{dS_n}{dt} = h \frac{\partial S_n}{\partial t} + \mathbf{q} \cdot \nabla S_n = 0 \quad (3.231)$$

$$h \frac{dS_n}{dt} - \nabla \cdot [h \mathbf{K} \cdot \nabla S_n] = [M_n^s + R_n - D_n] - [SS + R - I] S_n \quad n \in [1, N_s] \quad (3.232)$$

For the continuity equation of bed sediment:

$$\frac{\partial M_n}{\partial t} = D_n - R_n \quad n \in [1, N_s] \quad (3.233)$$

For the continuity equation of dissolved chemical:

$$h \frac{dC_i^w}{dt} = h \frac{\partial C_i^w}{\partial t} + \mathbf{q} \cdot \nabla C_i^w = 0 \quad (3.234)$$

$$\begin{aligned} & h \frac{dC_i^w}{dt} - \nabla \cdot [h \mathbf{K} \cdot \nabla C_i^w] \\ &= \sum_{m=1}^{N_{rx}} (a_{mj}^c - b_{mj}^c) k_m^{rb} h \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \right] \\ &+ \left[M_i^{cw} + h k_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} h (S_n C_{ni}^s) + \sum_{n=1}^{N_s} k_{ni}^{bb} (M_n C_{ni}^b) + M_i^{crw} - M_i^{ciw} \right] \\ &- \left[\lambda_i^c h + h k_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} + SS + R - I \right] C_i^w \quad i \in [1, N_c] \end{aligned} \quad (3.235)$$

For the continuity equation of particulate chemical on suspended sediment:

$$h \frac{d(S_n C_{ni}^s)}{dt} = h \frac{\partial (S_n C_{ni}^s)}{\partial t} + \mathbf{q} \cdot \nabla (S_n C_{ni}^s) = 0 \quad (3.236)$$

$$\begin{aligned} & h \frac{d(S_n C_{ni}^s)}{dt} - \nabla \cdot [h \mathbf{K} \cdot \nabla (S_n C_{ni}^s)] \\ &= \left[M_{ni}^{cs} + k_{ni}^{sf} h S_n C_i^w + \frac{R_n}{M_n} (M_n C_{ni}^b) - \frac{D_n}{S_n} (S_n C_{ni}^s) \right] - \left[\lambda_{ni}^s h + k_{ni}^{sb} h + SS + R - I \right] (S_n C_{ni}^s) \quad (3.237) \\ & \quad n \in [1, N_s], i \in [1, N_c] \end{aligned}$$

For the continuity equation of particulate chemical on bed sediment:

$$\begin{aligned} \frac{\partial (M_n C_{ni}^b)}{\partial t} &= \left[\frac{D_n}{S_n} (S_n C_{ni}^s) - \frac{R_n}{M_n} (M_n C_{ni}^b) + k_{ni}^{bf} M_n C_i^w \right] - \left[\lambda_{ni}^b + k_{ni}^{bb} \right] (M_n C_{ni}^b) \\ & \quad n \in [1, N_s], i \in [1, N_c] \end{aligned} \quad (3.238)$$

We solve the transport system by achieving the following steps.

- Step 1** Solve Eqs. (3.231), (3.234), and (3.236) to obtain the Lagrangian values for suspended sediments, dissolved chemicals, and particulate chemicals on suspend sediments.
- Step 2** Solve Eqs. (3.232) and (3.233) for S_n and M_n .

(a) Solve Eq. (3.232) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eq. (3.232))

=> Obtaining the *intermediate value* for suspended sediments.

(b) Prepare the corrector form of Eqs. (3.232) as described in Eq. (3.186). It can be written as follows.

$$\begin{aligned} h \frac{(S_n)^{N+1} - (S_n)^{N+1/2}}{\delta t} \\ = (RHS_n^s)^{N+1} - (RHS_n^s)^N \quad \left(\text{if } (RHS_n^s)^N \geq 0 \right) \\ = (RHS_n^s)^{N+1} - \frac{(RHS_n^s)^N}{(S_n)^N} (S_n)^{N+1/2} \quad \left(\text{if } (RHS_n^s)^N < 0 \right) \quad n \in [1, N_s] \end{aligned} \quad (3.239)$$

where

$$(RHS_n^s) = [M_n^s + R_n - D_n] - [SS + R - I] S_n \quad n \in [1, N_s] \quad (3.240)$$

(c) Solve Eq. (3.239) and Eq. (3.233) node by node with the Picard method to obtain the solutions for suspended and bed sediments.

Note: In Eqs. (3.232) and (3.233) both D_n and R_n need to be evaluated first, while in Eq. (3.232) K , h , R , I , and SS are either given or determined after the flow equations are solved. During each iteration in (c), both Eq. (3.239) and (3.233) are solved with the time-implicit scheme.

Step 3 Solve Eqs. (3.235), (3.237), and (3.238) for C_i^w , C_{ni}^s , and C_{ni}^b .

(a) Solve Eqs. (3.235) and (3.237) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eqs. (3.235) and (3.237)).

(b) Prepare the corrector form of Eqs. (3.235) and (3.237) described in Eq. (3.186). They can be written as follows.

For dissolved chemicals:

$$\begin{aligned}
& h \frac{(C_i^w)^{N+1} - (C_i^w)^{N+1/2}}{\delta t} \\
& = (RHS_i^c)^{N+1} - (RHS_i^c)^N \quad \left(\text{if } (RHS_i^c)^N \geq 0 \right) \\
& = (RHS_i^c)^{N+1} - \frac{(RHS_i^c)^N}{(C_i^w)^N} (C_i^w)^{N+1/2} \quad \left(\text{if } (RHS_i^c)^N < 0 \right) \quad i \in [1, N_c]
\end{aligned} \tag{3.241}$$

where

$$\begin{aligned}
(RHS_i^c) & = \sum_{m=1}^{N_r} (a_{mj}^c - b_{mj}^c) k_m^{rb} h \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \right] \\
& + \left[M_i^{cw} + h k_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} h (S_n C_{ni}^s) + \sum_{n=1}^{N_s} k_{ni}^{bb} (M_n C_{ni}^b) + M_i^{crw} - M_i^{ciw} \right] \\
& - \left[\lambda_i^c h + h k_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} + SS + R - I \right] C_i^w \quad i \in [1, N_c]
\end{aligned} \tag{3.242}$$

For particulate chemicals on suspended sediments:

$$\begin{aligned}
& h \frac{(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2}}{\delta t} \\
& = (RHS_{ni}^s)^{N+1} - (RHS_{ni}^s)^N \quad \left(\text{if } (RHS_{ni}^s)^N \geq 0 \right) \\
& = (RHS_{ni}^s)^{N+1} - \frac{(RHS_{ni}^s)^N}{(C_{ni}^s)^N} (C_{ni}^s)^{N+1/2} \quad \left(\text{if } (RHS_{ni}^s)^N < 0 \right) \quad n \in [1, N_s], i \in [1, N_c]
\end{aligned} \tag{3.243}$$

where

$$\begin{aligned}
(RHS_{ni}^s) & = \left[M_{ni}^{cs} + k_{ni}^{sf} h S_n C_i^w + \frac{R_n}{M_n} (M_n C_{ni}^b) - \frac{D_n}{S_n} (S_n C_{ni}^s) \right] \\
& - \left[\lambda_{ni}^s h + k_{ni}^{sb} h + SS + R - I \right] (S_n C_{ni}^s) \quad n \in [1, N_s], i \in [1, N_c]
\end{aligned} \tag{3.244}$$

(c) Solve Eqs. (3.241), (3.243), and (3.238) node by node with the Newton-Raphson method.

Note: In Eqs. (3.235), (3.237), and (3.238) S_n and M_n are computed in Step 1, while h , K , reaction rate constants, stoichiometry, 1-st order decay constants, partial atmospheric pressure, and sources/sinks are either given or determined after the flow equations are solved. To achieve the (c) of Step 3, the following residual equations are constructed

For dissolved chemicals:

$$\begin{aligned}
 (RES_i^c) &= h \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t \left[(RHS_i^c)^{N+1} - (RHS_i^c)^N \right] \quad \left(\text{if } (RHS_i^c)^N \geq 0 \right) \\
 &= h \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t \left[(RHS_i^c)^{N+1} - \frac{(RHS_i^c)^N}{(C_i^w)^N} (C_i^w)^{N+1/2} \right] \quad \left(\text{if } (RHS_i^c)^N < 0 \right) \quad (3.245)
 \end{aligned}$$

$i \in [1, N_c]$

For particulate chemicals on suspended sediments:

$$\begin{aligned}
 (RES_{ni}^s) &= h \left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2} \right] - \delta t \left[(RHS_{ni}^s)^{N+1} - (RHS_{ni}^s)^N \right] \quad \left(\text{if } (RHS_{ni}^s)^N \geq 0 \right) \\
 &= h \left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2} \right] - \delta t \left[(RHS_{ni}^s)^{N+1} - \frac{(RHS_{ni}^s)^N}{(S_n C_{ni}^s)^N} (S_n C_{ni}^s)^{N+1/2} \right] \quad \left(\text{if } (RHS_{ni}^s)^N < 0 \right) \quad (3.246)
 \end{aligned}$$

$n \in [1, N_s], i \in [1, N_c]$

For particulate chemicals on bed sediments:

$$(RES_{ni}^b) = (M_n C_{ni}^b)^{N+1} - (M_n C_{ni}^b)^N - \Delta t (RHS_{ni}^b)^{N+1} \quad n \in [1, N_s], i \in [1, N_c] \quad (3.247)$$

The associated Jacobian elements are thus computed as shown in the following.

For dissolved chemicals:

$$\begin{aligned}
 \frac{\partial (RES_i^c)}{\partial (C_1^w)^{N+1}} &= \delta_{il} h + \delta_{il} \delta t \left[\lambda_i^c h + SS + R - I + h k_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} \right] - \\
 &\delta t \left[\sum_{m=1}^{N_{rx}} (a_{mi}^c - b_{mi}^c) h \left(k_m^{rb} b_{ml}^c (C_1^w)^{b_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{b_{mj}^c} - k_m^{rf} a_{ml}^c (C_1^w)^{a_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{a_{mj}^c} \right) \right] \quad (3.248)
 \end{aligned}$$

$i \in [1, N_c]$

$$\frac{\partial (RES_i^c)}{\partial (S_n C_{ni}^s)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sb} h \quad n \in [1, N_s], i \in [1, N_c], \quad (3.249)$$

$$\frac{\partial (RES_i^c)}{\partial (M_n C_{ni}^b)^{N+1}} = -\delta_{il} \delta t k_{ni}^{bb} \quad n \in [1, N_s], i \in [1, N_c] \quad (3.250)$$

For particulate chemicals on suspended sediments:

$$\frac{\partial(\text{RES}_{ni}^s)}{\partial(C_1^w)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sf} S_n h \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.251)$$

$$\frac{\partial(\text{RES}_{ni}^s)}{\partial(S_n C_{nl}^s)^{N+1}} = \delta_{il} h + \delta_{il} \delta t \frac{D_n}{S_n} + \delta_{il} \delta t [\lambda_{ni}^s h + k_{ni}^{sb} h + SS + R - I] \quad (3.252)$$

$n \in [1, N_s], \quad i \in [1, N_c]$

$$\frac{\partial(\text{RES}_{ni}^s)}{\partial(M_n C_{nl}^b)^{N+1}} = -\delta_{il} \delta t \frac{R_n}{M_n} \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.253)$$

For particulate chemicals on bed sediments:

$$\frac{\partial(\text{RES}_{ni}^b)}{\partial(C_1^w)^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bf} M_n \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.254)$$

$$\frac{\partial(\text{RES}_{ni}^b)}{\partial(S_n C_{nl}^s)^{N+1}} = -\delta_{il} \Delta t \frac{D_n}{S_n} \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.255)$$

$$\frac{\partial(\text{RES}_{ni}^b)}{\partial(M_n C_{nl}^b)^{N+1}} = \delta_{il} + \delta_{il} \Delta t \frac{R_n}{M_n} + \delta_{il} \Delta t [\lambda_{ni}^b + k_{ni}^{bb}] \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (3.256)$$

It is noted that if SS, and R are negative (i.e., sinks), they should not appear in Eqs. (3.248) and (3.252). Likewise, if I is positive (i.e., sink), it must not appear in the two equations.

3.6. Solving the 3-D subsurface transport equations

The strategy for solving 3-D subsurface transport equations is similar to that used to solve 1-D and 2-D transport equations: using the predictor-corrector method to handle mobile materials (the dissolved chemicals in this case) and solve the ordinary differential equations of chemical reactions in the corrector process. In the following, we are to go through the procedures of solving the 3-D transport system. Recall Eqs. (2.63) through (2.65) and express them in the Lagrangian form for mobile materials as follows.

(1) For dissolved chemicals:

$$\theta \frac{dC_i^w}{dt} = \theta \frac{\partial C_i^w}{\partial t} + \mathbf{V} \cdot \nabla C_i^w = 0 \quad (3.257)$$

$$\begin{aligned}
& \theta \frac{DC_j^w}{Dt} - \nabla \cdot (\theta \mathbf{D} \cdot \nabla C_j^w) \\
& = q[C_j^{\text{in}} - C_j^w] - \lambda_j^c \theta C_j^w - \sum_{m=1}^{N_{rx}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{rf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} - k_m^{rb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \right] \quad (3.258) \\
& - \sum_{m=1}^{N_{rxs}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_c]
\end{aligned}$$

(2) For adsorbing sites:

$$\begin{aligned}
& \frac{\partial(\theta S_j)}{\partial t} \\
& = -\lambda_j^s \theta S_j - \sum_{m=1}^{N_{rxs}} a_{mj}^s \theta \left[k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_s] \quad (3.259)
\end{aligned}$$

(3) For adsorbed chemical:

$$\begin{aligned}
& \frac{\partial(\theta D_j)}{\partial t} \\
& = -\lambda_j^d \theta D_j + \sum_{m=1}^{N_{rxs}} b_{mj}^d \theta \left[k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_d] \quad (3.260)
\end{aligned}$$

We solve the transport system by achieving the following steps.

Step 1 Solve Eq. (3.257) to obtain the Lagrangian values for dissolved chemicals.

Step 2 Solve Eqs. (3.258), (3.259), and (3.260) for C_j^w , S_j , and D_j .

(a) Solve Eq. (3.258) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eq. (3.258)).

(b) Prepare the corrector form of Eqs. (3.258) as described in Eq. (3.186). It can be written as follows.

For dissolved chemicals:

$$\begin{aligned}
& \theta \frac{(C_i^w)^{N+1} - (C_i^w)^{N+1/2}}{\delta t} \\
& = (RHS_i^c)^{N+1} - (RHS_i^c)^N \quad \left(\text{if } (RHS_i^c)^N \geq 0 \right) \\
& = (RHS_i^c)^{N+1} - \frac{(RHS_i^c)^N}{(C_i^w)^N} (C_i^w)^{N+1/2} \quad \left(\text{if } (RHS_i^c)^N < 0 \right) \quad i \in [1, N_c]
\end{aligned} \tag{3.261}$$

where

$$\begin{aligned}
& (RHS_i^c) \\
& = q[C_j^{in} - C_j^w] - \lambda_j^c \theta C_j^w - \sum_{m=1}^{N_{rx}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{rf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} - k_m^{rb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \right] \\
& - \sum_{m=1}^{N_{rxs}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_c]
\end{aligned} \tag{3.262}$$

(c) Solve Eqs. (3.259), (3.260), and (3.261) node by node with the Newton-Raphson method.

Note: In Eqs. (3.258), (3.259), and (3.260) θ , D , reaction rate constants, stoichiometry, 1-st order decay constants, and sources/sinks are either given or determined after the flow equations are solved.

To achieve the (c) of Step 2, the following residual equations are constructed.

For dissolved chemicals:

$$\begin{aligned}
& (RES_i^c) \\
& = \theta [(C_i^w)^{N+1} - (C_i^w)^{N+1/2}] - \delta t [(RHS_i^c)^{N+1} - (RHS_i^c)^N] \quad \left(\text{if } (RHS_i^c)^N \geq 0 \right) \\
& = \theta [(C_i^w)^{N+1} - (C_i^w)^{N+1/2}] - \delta t \left[(RHS_i^c)^{N+1} - \frac{(RHS_i^c)^N}{(C_i^w)^N} (C_i^w)^{N+1/2} \right] \quad \left(\text{if } (RHS_i^c)^N < 0 \right)
\end{aligned} \tag{3.263}$$

$i \in [1, N_c]$

For adsorbing sites:

$$(RES_j^s) = (\theta S_j)^{N+1} - (\theta S_j)^N - \Delta t (RHS_j^s)^{N+1} \quad j \in [1, N_s] \tag{3.264}$$

in which

$$\begin{aligned} \text{RHS}_j^s &= -\lambda_j^s \theta S_j - \sum_{m=1}^{N_{\text{rxs}}} a_{mj}^s \theta \left[k_m^{\text{sf}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{\text{sb}} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_s] \end{aligned} \quad (3.265)$$

For adsorbed chemicals:

$$(\text{RES}_j^d) = (\theta D_j)^{N+1} - (\theta D_j)^N - \Delta t (\text{RHS}_j^d)^{N+1} \quad j \in [1, N_d] \quad (3.266)$$

in which

$$\begin{aligned} \text{RHS}_j^d &= -\lambda_j^d \theta D_j + \sum_{m=1}^{N_{\text{rxs}}} b_{mj}^d \theta \left[k_m^{\text{sf}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{\text{sb}} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_d] \end{aligned} \quad (3.267)$$

The associated Jacobian elements are thus computed as shown in the following.

For dissolved chemicals:

$$\begin{aligned} \frac{\partial(\text{RES}_i^c)}{\partial(C_1^w)^{N+1}} &= \delta_{i1} \theta + \delta_{i1} \delta t \left(\lambda_i^c \theta + q \right) \\ &- \delta t \left[\sum_{m=1}^{N_{\text{rx}}} (a_{mi}^c - b_{mi}^c) \theta \left(k_m^{\text{rb}} b_{mi}^c (C_1^w)^{b_{mi}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{b_{mj}^c} - k_m^{\text{rf}} a_{mi}^c (C_1^w)^{a_{mi}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{a_{mj}^c} \right) \right. \\ &+ \sum_{m=1}^{N_{\text{rxs}}} (a_{mi}^c - b_{mi}^c) \theta \left(k_m^{\text{sb}} b_{mi}^c (C_1^w)^{b_{mi}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right. \\ &\left. \left. - k_m^{\text{sf}} a_{mi}^c (C_1^w)^{a_{mi}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} \right) \right] \quad i \in [1, N_c] \end{aligned} \quad (3.268)$$

$$\frac{\partial(\text{RES}_i^c)}{\partial(S_1)^{N+1}} = \delta t \sum_{m=1}^{N_{\text{rxs}}} (a_{mi}^c - b_{mi}^c) \theta k_m^{\text{sf}} a_{mi}^s (S_1)^{a_{mi}^s-1} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1, j \neq 1}^{N_s} (S_j)^{a_{mj}^s} \quad i \in [1, N_c] \quad (3.269)$$

$$\frac{\partial(\text{RES}_i^c)}{\partial(D_1)^{N+1}} = -\delta t \sum_{m=1}^{N_{\text{rxs}}} (a_{mi}^c - b_{mi}^c) \theta k_m^{\text{sb}} b_{mi}^d (D_1)^{b_{mi}^d-1} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1, j \neq 1}^{N_d} (D_j)^{b_{mj}^d} \quad i \in [1, N_c] \quad (3.270)$$

For adsorbing sites:

$$\frac{\partial(\text{RES}_i^s)}{\partial(C_1^w)^{N+1}} = -\Delta t \sum_{m=1}^{N_{\text{rxs}}} a_{mi}^s \theta \left[k_m^{sb} b_{ml}^c (C_1^w)^{b_{ml}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right. \\ \left. - k_m^{sf} a_{ml}^c (C_1^w)^{a_{ml}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} \right] \quad i \in [1, N_s] \quad (3.271)$$

$$\frac{\partial(\text{RES}_i^s)}{\partial(S_1)^{N+1}} = \delta_{il} \theta + \delta_{il} \Delta t \theta \lambda_j^s \\ + \Delta t \left[\sum_{m=1}^{N_{\text{rxs}}} a_{mi}^s \theta k_m^{sf} a_{ml}^s (S_1)^{a_{ml}^s-1} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1, j \neq 1}^{N_s} (S_j)^{a_{mj}^s} \right] \quad i \in [1, N_s] \quad (3.272)$$

$$\frac{\partial(\text{RES}_i^s)}{\partial(D_1)^{N+1}} = -\Delta t \sum_{m=1}^{N_{\text{rxs}}} a_{mi}^s \theta k_m^{sb} b_{ml}^d (D_1)^{b_{ml}^d-1} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1, j \neq 1}^{N_d} (D_j)^{b_{mj}^d} \quad i \in [1, N_s] \quad (3.273)$$

For adsorbed chemicals:

$$\frac{\partial(\text{RES}_i^d)}{\partial(C_1^w)^{N+1}} = \Delta t \sum_{m=1}^{N_{\text{rxs}}} b_{mi}^d \theta \left[k_m^{sb} b_{ml}^c (C_1^w)^{b_{ml}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right. \\ \left. - k_m^{sf} a_{ml}^c (C_1^w)^{a_{ml}^c-1} \prod_{j=1, j \neq 1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} \right] \quad i \in [1, N_d] \quad (3.274)$$

$$\frac{\partial(\text{RES}_i^d)}{\partial(S_1)^{N+1}} = -\Delta t \sum_{m=1}^{N_{\text{rxs}}} b_{mi}^d \theta k_m^{sf} a_{ml}^s (S_1)^{a_{ml}^s-1} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1, j \neq 1}^{N_s} (S_j)^{a_{mj}^s} \quad i \in [1, N_d] \quad (3.275)$$

$$\frac{\partial(\text{RES}_i^d)}{\partial(D_1)^{N+1}} = \delta_{il} \theta + \delta_{il} \Delta t \theta \lambda_j^d \\ + \Delta t \sum_{m=1}^{N_{\text{rxs}}} b_{mi}^d \theta k_m^{sb} b_{ml}^d (D_1)^{b_{ml}^d-1} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1, j \neq 1}^{N_d} (D_j)^{b_{mj}^d} \quad i \in [1, N_d] \quad (3.276)$$

It is noted that if q is negative (i.e., sink), it should not appear in Eq. (3.268).

Section 4. EXAMPLES

In this section, we apply the model to perform fifteen simulations, including 1-D flow, 1-D transport, 1-D flow and transport, 2-D flow, 2-D transport, 2-D flow and transport, 3-D flow, 3-D transport, 3-D flow and transport, 1-D/2-D flow, 2-D/3-D flow, 1-D/2-D/3-D flow, 1-D/2-D flow and transport, 2-D/3-D flow and transport, and 1-D/2-D/3-D flow and transport. Unless specifically announced, the diffusion wave model is solved when the simulation of water flow is involved in those examples.

4.1. Examples of 1-D river/stream flow

4.1.1. Example 1 of 1-D river/stream flow

In this example, a horizontally 200 m-long river/stream containing a uniform width of 2 m is considered. The bottom elevation of the river/stream is shown in Figure 4.1. Manning's roughness is 0.015. Initially, it is dry everywhere. As the simulation starts, a uniform rainfall of 10^{-5} m/s covers the entire domain of interest. At the upstream boundary node (i.e., $X = 0$ m) water depth is set at 10^{-10} m, while at the downstream boundary node (i.e., $X = 200$ m) a water depth-dependent flow rate boundary condition is applied. No infiltration is considered in this example. The domain is discretized with twenty elements, 10 m long for each. A one-hour simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop.

Figures 4.2 and 4.3 plot water depth and discharge, respectively, at time = 100 s, 200 s, 300 s, 600 s, and 1200 s. Since the change of water depth is almost unobservable after time = 1200 s, a steady state is presumed to have reached thereafter under a uniform rainfall of 10^{-5} m/s. From Figure 4.2, a hydraulic jump is observed from $X = 50$ m to $X = 60$ m due to the slope change from -0.2 to -0.001. In each constant slope region (i.e., $X = 0$ to 50 m, $X = 50$ to 150 m, and $X = 150$ to 200 m), water depth has the tendency to increase gradually along the downslope direction because of a constant rainfall over the entire domain. We can also observe backwater effect in the region close to the downstream outlet ($X = 170$ to 200 m). In Figure 4.3, Discharge is computed by multiplying flow velocity with cross-sectional area which is water depth-dependent. In comparison of Figures 4.2 and 4.3, it is seen that the flow velocities within $X \in [150, 200]$ are large enough to make the discharge pattern different from the water depth pattern, which is due mainly to the 0.1 slope associated with this region.

4.1.2. Example 2 of 1-D river/stream flow

This example simulates water flow in a river/stream network system. The system is composed of three river/stream reaches that are connected through a junction (Figure 4.4). Each reach is 100 m long and is discretized with 11 nodes and 10 elements: Nodes 1 through 11 for Reach 1, 12 through 22 for Reach 2, and 23 through 33 for Reach 3. Nodes 11, 12, and 33 coincide with one another and are located at the junction. The junction covers the area between Nodes 10 and 11, Nodes 12 and 13, and Nodes 32 and 33.

Reaches 1 and 3 have a uniform river/stream width of 2 m and the slope of their bottom elevation is -0.2 along the downstream direction, while Reach 2 contains a uniform river/stream width of 3 m and the slope of its bottom elevation is -0.1. Manning's roughness is 0.02 for all three reaches. Initially, it is dry everywhere. As the simulation starts, a uniform rainfall of 10^{-5} m/s is put on Reach 1. At Node 1 water depth is kept at 0 m, while a constant flow of 2×10^{-4} m³/s flows through Node 23 through the simulation and a water

depth-dependent flow rate boundary condition is applied at the downstream boundary node (i.e., Node 22). No infiltration is considered in this example. A one-hour simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop.

Figures 4.5 through 4.7 plots water depth at various times for Reaches 1 through 3, respectively. Since rainfall and upstream boundary conditions do not vary with time, a steady state is observed after time = 600 s. It is noted that the downstream node of Reach 1 (i.e., at $X = 100$ m in Figure 4.5), the upstream node of Reach 2 (i.e., at $X = 0$ m in Figure 4.6) and the downstream node of Reach 3 (i.e., at $X = 100$ m in Figure 4.7) coincide with one another and are where the junction is. One can verify this by checking the water depths at these locations. We can see the marching of wet fronts in both Figures 4.6 and 4.7 and an increasing depth along the downstream direction in Figure 4.5 due to a constant uniform rainfall.

4.2. Example of 2-D overland flow

We give two examples in this subsection. Example 1 is to show the application of using the diffusion wave model to handle an overland system which contains the slope of bottom elevation ranging from 0.01 to 0.5; Because of the steep slope involved, the dynamic model is difficult to solve with any numerical scheme, even with the most physically natural method of characteristics. Example 2 is a standing wave problem to demonstrate the capability of the method of characteristics to accurately solve the dynamic wave model when the slope is small. Difficulty is encountered in dealing with water flow over steep slope overland system by solving the dynamic wave model. On the other hand, the diffusion wave model cannot provide accurate solution when the inertia terms are important, such as flow on a flat region. Thus, it is desirable to develop a hybrid model in which an adaptive scheme can be built to automatically select appropriate models (kinematic, diffusion, or dynamic wave models) for different regions of the entire watershed.

4.2.1. Example 1 of 2-D overland flow

The domain of interest covers a horizontal area of 200 m x 80 m. The bottom elevation contour is given in Figure 4.8. The domain is discretized with 320 triangular elements (Figure 4.9). Manning's roughness is 0.04. Initially, it is dry everywhere. A two-hour simulation is performed with a fixed time step size of 5 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop. As the simulation starts, a uniform rainfall of 10^{-5} m/s covers the entire domain of interest for the first half hour and 1.5×10^{-5} m/s for the third half hour. As for the second and the fourth half hours, the rainfall rate is zero. On the upstream boundary side (i.e., $X = 0$ m) water depth is set at 10^{-10} m through the simulation, while on the downstream boundary side (i.e., $X = 200$ m) a water depth-dependent flux boundary condition is applied. The boundaries of $Y = 0$ m and 80 m are impermeable. No infiltration is considered in this example.

Figure 4.10 plots water depth at various times from the simulation. From the figure, we can first see the irregular depth distribution due to the slope change of ground surface (Figure 4.8). Since the water depths at Time = 600 s, 1200 s, and 1800 s can not be distinguished, we may say a steady state has reached by Time = 600 s under a rainfall of 10^{-5} m/s. Likewise, the depths at the end of the second and the fourth half hours (i.e., Time = 3600 s and 7200 s, respectively) tells us the steady state for the two non-rainfall period of times have reached by then.

4.2.2. Example 2 of 2-D overland flow

A 1-D standing wave problem is considered in this example. It is solved by 2-D method of characteristics, as presented in Section 3.2.1. This problem is governed by the wave equations as follows.

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad (4.1)$$

$$\frac{\partial^2 \eta}{\partial t^2} = c^2 \frac{\partial^2 \eta}{\partial x^2} \quad (4.2)$$

$$c^2 = gh \quad (4.3)$$

where u is the velocity along the 1-D direction [L/T]; c is the wave speed [L/T]; h is water depth [L]; η is stage deviation [L]; g is gravity [L/T²]. The domain of interest is 200 m long in the x -direction and 50 m wide in the y -direction. It is discretized with 20 elements: 10 m x 50 m each. The boundary end of $X = 200$ m is closed, while the other one at $X = 0$ m is open and the water stage is forced up and down according to

$$\eta|_{x=0m} = \frac{1}{10} \sin \frac{2\pi t}{200} \quad (4.4)$$

Thus, we set $u = 0$ m/s at $X = 200$ m to settle the boundary condition for achieving the simulation. The analytical solution of this problem can be found as follows [Wang and Connor, 1975].

$$u = - \frac{a\sqrt{c}}{h \cos \frac{2\pi}{\sqrt{c}}} \sin \left[\frac{2\pi}{\sqrt{c}} \left(\frac{x}{200} - 1 \right) \right] \cos \frac{2\pi t}{200} \quad \text{m/s} \quad (4.5)$$

$$\eta = - \frac{a}{\cos \frac{2\pi}{\sqrt{c}}} \cos \left[\frac{2\pi}{\sqrt{c}} \left(\frac{x}{200} - 1 \right) \right] \sin \frac{2\pi t}{200} \quad \text{m} \quad (4.6)$$

A simulation of 400 seconds is performed, where time step size is set to 2.5 seconds. The initial condition is given at $t = 50$ s according to Eqs. (4.5) and (4.6). Figures 4.11 and 4.12 show the comparison of water depth and velocity, respectively, between analytical solution and computed results at various times. The comparison simply tells that the method of characteristics can solve the dynamic wave model quite accurately.

4.3. Example of 1-D river/stream transport

This example is to demonstrate the capability of the model in simulating both chemical and sediment transport. A horizontally 200 m-long river/stream containing a uniform width of 2 m is considered. To focus on transport, we assume water depth is 2 m and river/stream velocity is 1 m/s throughout the river/stream. Three dissolved chemicals are considered to undergo the following reaction.

$$\overline{C1} + \overline{C2} \rightleftharpoons \overline{C3} \quad k_f = 0.002, \quad k_b = 0.005 \quad (4.7)$$

where $\overline{C1}$, $\overline{C2}$, and $\overline{C3}$ represent dissolved chemicals.

Three sizes of sediments are taken into account and are considered to be cohesive sediments. The settling speeds are 1.2×10^{-6} m/s for Sediment 1, 1.5×10^{-4} m/s for Sediment 2, and 4.5×10^{-2} m/s for Sediment 3. The critical shear stresses for deposition and erosion are $2.75 \text{ g/m}^2\text{s}$ and $2.68 \text{ g/m}^2\text{s}$, respectively, for all three sediments. The following sorption reactions are included.

$$\overline{CC} + \overline{SS1} \rightleftharpoons \overline{PS1} + \overline{SS1} \quad k_f = 0.001, \quad k_b = 0.0 \quad (4.8)$$

$$\overline{CC} + \overline{SS2} \rightleftharpoons \overline{PS2} + \overline{SS2} \quad k_f = 0.001, \quad k_b = 0.0 \quad (4.9)$$

$$\overline{CC} + \overline{SS3} \rightleftharpoons \overline{PS3} + \overline{SS3} \quad k_f = 0.001, \quad k_b = 0.0 \quad (4.10)$$

$$\overline{CC} + \overline{BS1} \rightleftharpoons \overline{PB1} + \overline{BS1} \quad k_f = 0.0001, \quad k_b = 0.0 \quad (4.11)$$

$$\overline{CC} + \overline{BS2} \rightleftharpoons \overline{PB2} + \overline{BS2} \quad k_f = 0.0001, \quad k_b = 0.0 \quad (4.12)$$

$$\overline{CC} + \overline{BS3} \rightleftharpoons \overline{PB3} + \overline{BS3} \quad k_f = 0.0001, \quad k_b = 0.0 \quad (4.13)$$

where \overline{CC} can be $\overline{C1}$, $\overline{C2}$, or $\overline{C3}$; $\overline{SS1}$, $\overline{SS2}$, and $\overline{SS3}$ are suspended sediments; $\overline{BS1}$, $\overline{BS2}$, and $\overline{BS3}$ are bed sediments; $\overline{PS1}$, $\overline{PS2}$, and $\overline{PS3}$ are particulate chemicals on suspended sediments associated with \overline{CC} ; $\overline{PB1}$, $\overline{PB2}$, and $\overline{PB3}$ are particulate chemicals on bed sediments associated with \overline{CC} . We have, therefore, 18 sorption reactions in total.

Initially, only bed sediments exist in the domain of interest. The initial concentration is 50 g/m^3 for the first bed sediment, 75 g/m^3 for the second, and 100 g/m^3 for the third. As the simulation starts, Dirichlet boundary conditions are applied to the upstream boundary node (i.e., $X = 0 \text{ m}$), where all dissolved chemicals have a constant concentration of 1 g/m^3 and all other mobile materials have zero concentration at this boundary node. The longitudinal dispersivity is 0.01 m . A 1000 second simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for both linear and nonlinear iterations involved in the computation.

Figures 4.13 through 4.17 plot the numerical results at various time, including concentration distributions for (1) dissolved chemicals (Figure 4.13), (2) suspended sediments (Figure 4.14), (3) bed sediments (Figure 4.15), (4) particulate chemicals on suspended sediments (Figure 4.16), and (5) particulate chemicals on bed sediments (Figure 4.17). Since the first and second dissolved chemicals are involved in identical reactions, their concentration distributions are identical to each other, so do those of their related particulate chemicals.

Figure 4.13 shows a decreasing dissolved chemical concentration for all three dissolved chemicals. This is because we allow the adsorption to happen, but do not allow desorption from particulate chemicals to dissolved chemicals (see Eqs. (4.8) through (4.13)). Figure 4.14 shows the trend of increasing concentration of suspended sediment along the downstream direction, while Figure 4.15 depict the decrease of bed sediment with the increase of time. Figures 4.14 and 4.15 tell that the deposition is less than the erosion under the condition set for this example. Figures 4.16 and 4.17 also help verify this. Since the dissolved chemicals are little in the downstream region, the major source of chemicals are the particulate chemicals on suspended sediments that are transported from the upstream region along with water. Because

erosion is greater than deposition, we can hardly find particulate chemicals on bed sediments in the downstream region (Figure 4.17). On the other hand, we observe an increase of particulate chemical on suspended sediments along the downstream direction (Figure 4.16). By comparing the numerical results at various times, it seems that the concentration distributions (Figures 4.13, 4.14, and 4.16) are approaching a steady state. This tendency will continue until the bed sediments are completely depleted, starting from the upstream end.

4.4. Example of 2-D overland transport

The domain of interest has covered a horizontal area of 200 m x 70 m and is discretized with 140 rectangular elements: 10 m x 10 m for each element. To deal with transport only, water depth is set to 1 m and the velocity is -1.0 m/s in the x-direction and 0.0 m/s in the y-direction everywhere. The following chemical reactions are embraced.

$$\overline{C1} + \overline{C2} \rightleftharpoons \overline{C4} \quad k_f = 0.01, \quad k_b = 0.005 \quad (4.14)$$

$$\overline{C1} + \overline{C3} \rightleftharpoons \overline{C5} \quad k_f = 0.01, \quad k_b = 0.0025 \quad (4.15)$$

$$\overline{C2} + 2\overline{C3} \rightleftharpoons \overline{C6} \quad k_f = 0.01, \quad k_b = 0.001 \quad (4.16)$$

where $\overline{C1}$, $\overline{C2}$, $\overline{C3}$, $\overline{C4}$, $\overline{C5}$, and $\overline{C6}$ are dissolved chemicals.

Initially, there is no dissolved chemical anywhere in the domain. A 600 second simulation is performed with a fixed time step size of 10 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop. As the simulation starts, a Dirichlet concentration of 1 g/m³ is applied for $\overline{C1}$, $\overline{C2}$, and $\overline{C3}$ on the upstream boundary (i.e., X = 200 m) between Y = 30 m and 40 m. The boundaries of Y = 0 m and 70 m are impervious. The longitudinal and transverse dispersivities are 0.5 m and 0.1 m, respectively. The diffusion coefficient is 10^{-5} m²/s.

Figures 4.18 through 4.23 show the numerical result at time = 260 s. A steady state result is considered to have reached after 260 s. The maximum concentrations of $\overline{C4}$, $\overline{C5}$, and $\overline{C6}$ are 0.26286 g/m³, 0.25637 g/m³, and 0.16833 g/m³, respectively, which are found in the middle of downstream area (i.e., X = 40 to 50 m and Y = 30 to 40 m).

4.5. Example of 1-D river/stream flow and transport

In this example, a horizontally 200 m-long river/stream containing a uniform width of 2 m is considered. The bottom elevation of the river/stream is shown in Figure 4.1. Manning's roughness is 0.015. Initially, it is dry everywhere. The chemical reactions considered are identical to those in the example of 2-D transport (Eqs. (4.14) through (4.16)). As the simulation starts, a uniform rainfall of 10^{-5} m/s covers the entire domain of interest, which contains the first three chemicals (i.e., $\overline{C1}$, $\overline{C2}$, and $\overline{C3}$) of 1 g/m³. At the upstream boundary node (i.e., X = 0 m) water depth is kept at 10^{-10} m and the concentrations are kept at 1 g/m³ for $\overline{C1}$, $\overline{C2}$, $\overline{C3}$ and at 0 g/m³ for $\overline{C4}$, $\overline{C5}$, $\overline{C6}$. At the downstream boundary node (i.e., X = 200 m) a water depth-dependent flow rate boundary condition is employed for flow and a variable boundary condition is applied for transport. Infiltration is neglected. The domain is discretized with twenty

elements, 10 m long for each. A one-hour simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for required iteration in both flow and transport computations.

Figure 4.24 depicts water depth at various times for the simulation. It is the same as Figure 4.2 because they have an identical setup for the flow simulation and we assume the flow is not influenced by transport in the model. Figures 4.25 through 4.31 show the concentration distributions at various times for the first through the sixth dissolved chemicals, respectively. It is seen that the third dissolved chemicals are consumed most among the three reactant chemicals that consumes most in this example (Figures 4.25 through 4.27). This is because all three reactions contain the same forward reaction rate constant (Eqs. (4.16) through (4.18)) but the third reaction has the smallest backward reaction rate constant and the third dissolved chemical has a stoichiometric coefficient of 2 as a reactant chemical in the third reaction (Eq. (4.16)).

4.6. Example of 2-D overland flow and transport

The setup for the flow simulation in this example is the same as that in the example of 2-D flow (Section 4.2) except that time step size is 2.5 s for this example. The same chemical system as described in both Sections 4.4 and 4.5 is also considered here. Initially, it is dry and there is no chemical in the domain of interest. As the simulations starts, Dirichlet boundary conditions are applied on the upstream boundary (i.e., $X = 0$ m) for the transport simulation, where the concentrations of \bar{C}_1 , \bar{C}_2 , \bar{C}_3 are maintained at 1 g/m^3 and those of \bar{C}_4 , \bar{C}_5 , \bar{C}_6 are at 0 g/m^3 .

Figures 4.31 through 4.37 plot the numerical results at various times. Figure 4.31 is actually representing the same computational result as Figure 4.10 for Example 1 of 2-D overland flow in Section 4.2.1. This is again because this example has a simulation setup identical to that of the example in Section 4.2.1 and the feedback from transport to flow is not considered in the model. Although the results shown in Figures 4.32 through 4.37 are difficult to analyze, we can observe the same concentration distribution trends from upstream to downstream for the six dissolved chemicals as those shown in Figures 4.25 through 4.30. Additionally, it is consistent that \bar{C}_3 and \bar{C}_6 are the chemicals having the smallest concentration among the three reactant chemicals and the three product chemicals, respectively, in the downstream region.

4.7. Example of 1-D/2-D flow

A flow system including both 1-D river/stream and 2-D overland is considered in this section. The topography and discretization of the system is plotted in Figure 4.38. As shown in the figure, water would flow from overland into the river/stream that is located in the middle of the system (i.e., the blue strip) and then leave the system through the downstream outlet of the river/stream (i.e., at $X = 0$ m, $Y = 0$ m). The slope of river/stream bottom elevation is 0.02.

The river/stream width increases along river/stream's downstream direction: 10 m at $Y = 100$ and 90 m, 12 m at $Y = 80$ and 70 m, 14 m at $Y = 60$ and 50 m, 16 m at $Y = 40$ and 30 m, 18 m at $Y = 20$ and 10 m, and 20 m at the outlet (i.e., $Y = 0$ m). The width changes linearly between any two consecutive locations mentioned above. The system is initially dry. A variable rainfall is applied to the system during a two-hour simulation, which is $5 \times 10^{-7} \text{ m/s}$ during the first twenty minutes, $1 \times 10^{-6} \text{ m/s}$ between 20 and 40 minutes, $2 \times 10^{-6} \text{ m/s}$ between 40 and 60 minutes, no rainfall between 60 and 80 minutes, $4 \times 10^{-6} \text{ m/s}$ between 80 and 100 minutes, and $5 \times 10^{-7} \text{ m/s}$ for the last twenty minutes of the simulation. A constant water depth of 0 m is set

at the ridge top of the system during the simulation. A water depth-dependent flux boundary condition is employed on the interface between 2-D overland and 1-D river/stream to determine the injection of water from overland to river/stream. Impermeable boundary condition is employed for the overland boundary at $Y = 0$ m ($X = -400$ to -10 m and $X = 10$ to 400 m). The upstream end of the river/stream is treated as a junction, where water budget is used to determine the water depth there. A water depth-dependent flow rate boundary condition is used to compute the water going out from the river/stream downstream boundary, which is also the only outlet of the system. The time step size for 2-D overland flow computation is 20 seconds and it is 2 seconds for calculating 1-D river/stream flow (i.e., 1 2-D time step = 10 1-D time steps).

Figures 4.39 and 4.40 plot water depth and velocity, respectively, at various times for 1-D river/stream along the river downstream (i.e., from $Y=1000$ m to $Y=0.0$ m). Figure 4.41 depicts the contour of water depth at various times for 2-D overland. From Figure 4.39, we can easily observe the back water effect due to the depth-dependent flow rate at the outlet of 1-D river/stream. Also, we see that the junction (at $X = 0$ m in Figures 3.39 and 3.40) collects water from the converging overland flow and has the largest water depth in the river/stream. This seems contradictory to our intuition. However, such a result is the consequence of the widening of river width from upstream to downstream and a relatively flat river bottom. Figure 4.41 illustrates how water depth changes with rainfall rates in the overland domain. We can also observe the back water effect due to the depth-dependent normal flux given on the river/stream- and junction-related downstream boundary (i.e., the 1-D/2-D interface boundary).

4.8. Example of 1-D/2-D flow and transport

This example considers both flow and transport in 1-D river/stream and 2-D overland. The topography and grids are shown in Figure 4.42 where flow is driven into the river/stream from the overland simply due to gravity. The slope of river bottom elevation is 0.01. The river/stream has a uniform width of 10 m. The system is initially dry. A variable rainfall is applied to the system during a two-hour simulation, which is 10^{-5} m/s during the first twenty minutes, 2×10^{-5} m/s between 20 and 40 minutes, 10^{-5} m/s between 40 and 60 minutes, 2×10^{-5} m/s between 60 and 80 minutes, 10^{-5} m/s between 80 and 100 minutes, and no rainfall for the last twenty minutes of the simulation. A constant water depth of 10^{-4} m is set at the ridge top of the system during the simulation. A water depth-dependent flux boundary condition is employed on the interface between 2-D overland and 1-D river/stream to determine the injection of water from overland to river/stream. Impermeable boundary condition is employed for the overland boundary at $Y = 0$ m and $Y = 900$ m ($X = 200$ to 595 m and $X = 605$ to 1000 m). Water depth is maintained at 10^{-3} m at the upstream end of the river/stream. A water depth-dependent flow rate boundary condition is used to compute the water going out from the river/stream downstream boundary. Manning's roughness is 0.01 for overland and 0.03 for river/stream. The time step size for 2-D overland flow computation is 10 seconds and it is 2 seconds for calculating 1-D river/stream flow.

As for the transport simulation, six dissolved chemicals and two reactions are taken into account. Among the six chemicals, five of them are involved in the two reactions as described in the following and the other one is non-reactive.

$$\overline{C1} + \overline{C2} \rightleftharpoons \overline{C4} \quad k_f = 0.01, \quad k_b = 0.005 \quad (4.17)$$

$$\overline{C1} + \overline{C3} \rightleftharpoons \overline{C5} \quad k_f = 0.01, \quad k_b = 0.005 \quad (4.18)$$

The dissolved chemical $\overline{C5}$ is radioactive and the decay constant is 10^{-4} 1/s. $\overline{C1}$, $\overline{C2}$, $\overline{C3}$,

and $\overline{C6}$ exist in rainfall with a constant concentration of 1 g/m^3 . In 2-D overland transport, variable boundary conditions are applied on both the upstream boundary (i.e., ridge top), where the concentration is 1 g/m^3 for $\overline{C1}$, $\overline{C2}$, $\overline{C3}$, and $\overline{C6}$, and is 0 g/m^3 for the other two chemicals if the flow is directed into the domain of interest. For the overland-river interface, we also apply variable boundary conditions by using the respective concentrations in the channel as the incoming concentrations when the flow is directed from river/stream to overland on the interface boundary. As for 1-D river/stream transport, the same variable boundary condition as is employed for the overland ridge top is applied to both the upstream and the downstream boundary nodes (i.e., located at (600 m, 900 m) and (600 m, 0 m), respectively).

Figure 4.43 plots water depth at various times for 1-D river/stream along the river downstream. Figure 4.44 plots water depth at various times for 2-D overland. Figures 4.45 through 4.50 depict the concentration of the first through the sixth dissolved chemicals, respectively, at various times for 1-D transport. Figures 4.51 through 4.56 show the concentration of the first through the sixth dissolved chemicals, respectively, at various times for 2-D overland.

Both Figures 4.43 and 4.44 indicate that steady state have been reached by the end of each constant rainfall period of time (each rainfall period lasts for twenty minutes). For both 1-D and 2-D flows, the back water effect is obvious. The reason has been given in the previous example. Figures 4.50 and 4.56 show the uniformly distributed concentration of the nonreactive dissolved chemical in 1-D and 2-D, respectively. This numerical result help to verify our model when 1-D flow, 2-D flow, 1-D transport, and 2-D transport are all taken into account.

Since the second and the third dissolved chemicals are involved in identical aqueous complexation reactions, they should have the same concentration distribution, so should their respective product chemicals (i.e., the fourth and the fifth chemicals, respectively). However, the radioactive nature of the fifth chemical makes the difference between them as well as the difference between their respect product chemicals. On the other hand, the decay is so slow so that the difference mentioned above is almost invisible (compare Figures 4.46 with 4.47, Figures 4.48 with 4.49, Figures 4.52 with 4.53, and Figures 4.54 with 4.55).

4.9. Example of 3-D subsurface flow

This example was designed to demonstrate a 3-D flow simulation with the 3DFEMWATER model [Yeh and Cheng, 1993]. Since the computational results from our watershed model matches that from 3DFEMWATER perfectly, we have verified the 3-D subsurface flow module with this example. The description of the example is as follows. The example involves the steady flow to a pumping well where the total head is maintained at 30 m during pumping. The region of interest is bounded on the left ($x = 0 \text{ m}$) and right ($x = 1000 \text{ m}$) by hydraulically connected rivers; on the front ($y = -400 \text{ m}$), back ($y = 400 \text{ m}$), and bottom ($z = 0 \text{ m}$) by impervious aquifuges; and on the top ($z = 72 \text{ m}$) by an air-soil interface. The pumping well is located at (540,0). The water table is assumed to be horizontal and is 60 m above the bottom of the aquifer before pumping. The saturated hydraulic conductivity has components $K_{xx} = 5 \text{ m/d}$, $K_{yy} = 0.5 \text{ m/d}$, and $k_{zz} = 2 \text{ m/d}$. The porosity of the medium is 0.25 and the field capacity is 0.0125. The following two equations are taken to describe the unsaturated hydraulic properties.

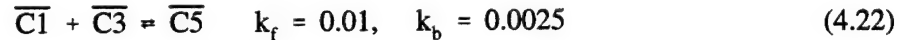
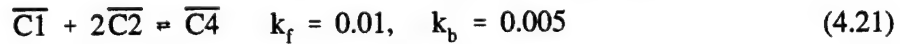
$$\theta = \theta_r + (\theta_s - \theta_r) \frac{1}{1 + (\alpha |h_a - h|)^{\beta}} \quad (4.19)$$

$$K_r = \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^2 \quad (4.20)$$

where θ_s is porosity; θ_r is the minimum moisture content that is associated with the minimum pressure head h_a ; α and β are parameters used to compute the moisture content and relative hydraulic conductivity. Because of the symmetry, the region for numerical simulation is taken as $x \in [0 \text{ m}, 1000 \text{ m}]$, $y \in [0 \text{ m}, 400 \text{ m}]$, $z \in [0 \text{ m}, 72 \text{ m}]$, the boundary condition are given as: pressure head is assumed hydrostatic on two vertical planes at (1) $x = 0 \text{ m}$ and $z \in [0 \text{ m}, 60 \text{ m}]$ and (2) $x = 1000 \text{ m}$ and $z \in [0 \text{ m}, 60 \text{ m}]$; no flux is imposed on all other boundaries of the flow regime. The steady-state solution corresponding to the above boundary conditions is sought with the pressure head error tolerances of 0.01 m and 0.005 m as the criteria to determine convergence for nonlinear iterations and linear matrix solvers, respectively. The steady-state solution is plotted in Figure 4.57.

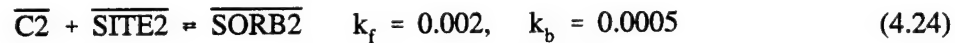
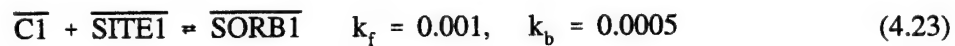
4.10. Example of 3-D subsurface transport

This example is to demonstrate the capability of the model in simulating kinetics chemical transport in a 3-D domain. A 1000 cm long, 100 cm wide, and 40 cm deep region is considered. It is discretized with nonuniform hexahedral elements (Figure 4.58). To focus on transport, we assume a constant effective porosity of 0.3 throughout the entire domain that is saturated. The Darcy velocity (specific discharge) is 0.3 cm/minute. Three dissolved chemicals are considered to undergo the following reaction.



where $\overline{C1}$, $\overline{C2}$, $\overline{C3}$, $\overline{C4}$, and $\overline{C5}$ represent dissolved chemicals.

The following adsorption reactions, with two adsorbing sites and two adsorbed chemicals involved, are also considered.



where $\overline{\text{SITE1}}$ and $\overline{\text{SITE2}}$ are adsorbing sites; $\overline{\text{SORB1}}$ and $\overline{\text{SORB2}}$ are adsorbed chemicals.

Initially, there contain no dissolved chemicals, nor adsorbed chemicals. Only are adsorbing sites in the domain of interest. The initial concentration is 0.1 g/cm³ for both adsorbing sites. The boundary conditions for the transient simulation are: no flux for the top ($z = 40 \text{ cm}$), the bottom ($z = 0 \text{ cm}$), the front ($y = 0 \text{ cm}$) and the back ($y = 100 \text{ cm}$) boundaries; flow-out variable boundary condition (or zero Neumann flux) for the downstream boundary ($x = 1000 \text{ cm}$); Dirichlet boundary conditions applied to the boundary nodes included in the patch area of $y \in [30 \text{ cm}, 70 \text{ cm}]$ and $z \in [16 \text{ cm}, 24 \text{ cm}]$ on the upstream boundary ($x = 0 \text{ cm}$) where a constant concentration of 1 g/cm³ are maintained for the first three dissolved chemicals and zero concentration is set for the other two dissolved chemicals; flow-in variable boundary condition with zero concentration for the upstream boundary area that is not included in the aforementioned patch. The longitudinal dispersivity is 0.01 cm, the transverse dispersivity is 0.001 cm, and the molecular diffusion

coefficient is 10^{-5} cm²/minute. A 60 hour simulation is performed with a fixed time step size of 10 minutes. A relative error of 10^{-4} is used to determine convergence for both linear and nonlinear iterations involved in the computation.

Figures 4.59 through 4.62 depict the numerical results at the end of simulation for $\overline{C1}$, $\overline{C4}$, $\overline{SITE1}$, and $\overline{SORB1}$, respectively. In each figure, we plot the concentration contours on the planes of $y = 50$ cm and $z = 20$ cm for clear views for readers to visualize. The results shown on these figures provide not only the qualitative description of what is happening in the system, which we can expect from the chemical reactions taken into account and from the boundary conditions set for the simulation, but a quantitative analysis on the concentration distribution at time = 60 hours. The highest concentration of $\overline{C1}$ is 1.0 g/cm³ which is the given Dirichlet boundary condition at nodes in the patch area on the upstream boundary because the reactions involving $\overline{C1}$ (i.e., Eqs. (4.21) through (4.23)) cause the consumption of $\overline{C1}$ when it enters the domain along with the flow. The highest concentration is 0.21153 g/cm³ at (210, 50, 20) for $\overline{C4}$, which results from its production through aqueous complexation (Eq. (4.21)) and the decreasing of both $\overline{C1}$ and $\overline{C2}$ along the x-direction. On the upstream boundary patch, the highest concentration of $\overline{SORB1}$ (0.0663652 g/cm³) and the lowest concentration of $\overline{SITE1}$ (0.033634 g/cm³) are found due to the adsorption (Eq. (4.23)).

4.11. Example of 3-D subsurface flow and transport

This example is to demonstrate the capability the model has to handle both 3-D subsurface flow and transport. In this example, the initial flow condition is computed by solving the steady-state flow governing equation based on the given boundary conditions, where an impermeable boundary condition is applied to the front ($y = 0$ m), back ($y = 100$ m), and bottom ($z = 0$ m) boundaries; a total head of 26 m is specified on the lower part of the left boundary ($x = 0$ m and $z \leq 26$ m); a total head of 13 m is specified on the lower part of the right boundary ($x = 1000$ m and $z \leq 13$ m); a variable boundary condition of zero ponding depth and zero rainfall flux is applied to the upper part of right and left boundaries; a variable boundary condition of zero ponding depth and a rainfall rate of 10^{-5} m/sec is used for the top boundary (i.e., the ground surface boundary) in the 6 hour transient simulation. In determining the initial steady-state flow condition, zero rainfall rate is employed for the top boundary. Figure 4.63 shows the domain and discretization for the simulation here. The saturated hydraulic conductivity has components $K_{xx} = 2 \times 10^{-4}$ m/s, $K_{yy} = 10^{-5}$ m/s, and $k_{zz} = 10^{-5}$ m/s. The following soil characteristic equations are used to describe the hydraulic properties in unsaturated zones.

$$\begin{aligned} \theta &= 0.3 & \text{if } 0 < h \\ \theta &= 0.15 + 0.0015(h + 100) & \text{if } -100 < h < 0 \\ \theta &= 0.15 & \text{if } h < -100 \end{aligned} \quad (4.25)$$

$$\begin{aligned} K_r &= 1 & \text{if } 0 < h \\ K_r &= \frac{h + 100}{100} & \text{if } -100 < h < 0 \\ K_r &= 0 & \text{if } h < -100 \end{aligned} \quad (4.26)$$

In the transport simulation the following reaction, with three dissolved chemicals involved, is

considered.

$$\overline{C1} + \overline{C2} = 2\overline{C3} \quad k_f = 0.01, \quad k_b = 0.001 \quad (4.27)$$

Initially, no chemicals exist in the domain. As the transient simulation starts, $\overline{C1}$ and $\overline{C2}$ of 1 g/m^3 are brought into the subsurface domain through rainfall on a part of the top boundary ($x \in [60 \text{ m}, 500 \text{ m}]$) and this is the only source that chemicals would enter the domain. To achieve the transient simulation associated with such a condition, we employ variable boundary conditions for the top, the right, and the left boundaries, with a concentration of 1 g/m^3 associated with the incoming flow for the 1st and 2nd dissolved chemicals on the restricted top boundary and a zero incoming concentration for the rest of the variable boundary and for the 3rd dissolved chemical. We also apply the no-flux condition for the front, the back, and the bottom boundaries. The time step size is 100 seconds for computing flow and is 5 seconds for computing chemical transport. In other words, one flow time step contains 20 transport time steps. An absolute error of 0.001 m is used to determine convergent flow solutions, while a relative error of 0.0001 is taken as the stopping criterion for solving both linear and nonlinear equations in the transport simulation.

Figures 4.64 through 4.66 plot the numerical results of pressure head, the concentration of the 1st (or the 2nd) dissolved chemical, and the concentration of the 3rd dissolved chemical, respectively, on the plane of $y = 50 \text{ m}$ at various times. At the end of simulation (time = 6 hours, Figure 4.64), we can observe unsaturated zones close to the upper part of the right and the left boundaries because infiltration, contributed only by rainfall, does not provide enough water to make saturation for the two parts. Since the part on the right has a low elevation, it should allow water to accumulate on ground surface through surface runoff after the subsurface cannot absorb rainfall completely at higher elevation. This missing of accounting for surface runoff can lead to errant simulation results in many cases. That is to say, the coupling of surface and subsurface systems is needed when surface runoff is not negligible. Without surface runoff taken into account, the migration of chemicals to the right boundary is slow (Figures 4.65 and 4.66). This also indicates a possibility of incorrect estimate on chemical distribution when only is the subsurface system considered. We will demonstrate different simulation results on both flow and chemical transport in Section 4.13, where the coupling of surface and subsurface systems is considered.

4.12. Example of 2-D/3-D flow

The domain of interest for this example is identical to that for the 3-D flow and transport example (Figure 4.63 in Section 4.11). The initial condition is also computed according to the boundary conditions the same as those in Section 4.11. The rainfall is $2 \times 10^{-5} \text{ m/s}$ during the 1st twenty minutes. Then rain stops for 1 hour, followed by a rainfall of 10^{-5} m/s for 1 hour and $1.5 \times 10^{-5} \text{ m/s}$ afterwards till the end of simulation (time = 6 hours). The water depth is set to zero for the highest location of the 2-D overland domain (i.e., at $x = 0 \text{ m}$), while a depth-dependent flux is given for the boundary condition at the lowest location (i.e., at $x = 1000 \text{ m}$). The rest of the overland boundary is assumed no-flux (i.e., at $y = 0 \text{ m}$ and $y = 100 \text{ m}$). The water depth computed from 2-D overland flow is used as the ponding depth for implementing the variable boundary condition on the top boundary of 3-D subsurface flow. The remaining boundary conditions for computed 3-D subsurface flow are set identical to those in Section 4.11. A relative error of 10^{-4} is used to determine convergence for 2-D overland flow, and an absolute error of 10^{-3} m is employed to identify a convergent solution of 3-D subsurface flow. The time step sizes for 3-D and 2-D computation are 100 seconds and 2 seconds, respectively.

Figure 4.67 plots the depth of 2-D overland flow at various times and Figure 4.68 shows the pressure

head distribution on the $y = 50$ m plane at various times. From the top two graphs of Figure 4.67, it is obvious that the rainfall in the first twenty minutes is absolutely absorbed into 3-D subsurface. In the meantime, moisture content in the unsaturated zone (the blue band in Figure 4.68) increases with time due to this infiltration contribution. When rain stops, water drainage caused by gravity decreases moisture content in the unsaturated zone. As soon as rain is resumed, moisture content increases again, and saturated area expands in the uphill direction. Also, we can observe the accumulation of water on ground surface after the soil cannot accept all rainfall water (Figures 4.67 and 4.68). At the end of simulation (time = 6 hours), there is only a small unsaturated zone next to the highest location of the system.

4.13. Example of 2-D/3-D flow and transport

The flow conditions for this example is the same as those for the 2-D/3-D flow example in Section 4.12, except the rainfall is constant at 10^{-5} m/s during the 6 hour simulation period. There is one aqueous complexation reaction considered as follows.

$$\overline{C1} + 2\overline{C2} \rightleftharpoons \overline{C3} \quad k_f = 0.001, \quad k_b = 0.0001 \quad (4.28)$$

Initially, no chemicals exist in the domain. As the transient simulation starts, $\overline{C1}$ and $\overline{C2}$ of 1 g/m^3 exist in the rainfall that falls on a part of the overland surface ($x \in [60 \text{ m}, 500 \text{ m}]$), but do not appear in the precipitation falling onto the rest of overland surface. To achieve the transient simulation associated with such a condition, we employ surface/subsurface variable boundary conditions for the top boundary and a variable boundary condition with a zero incoming concentration for the right and left subsurface boundaries. We also apply the no-flux condition for the front, the back, and the bottom boundaries.

Variable time step sizes, 10 seconds from 0 to 40 seconds, 40 seconds from 40 to 200 seconds, 100 seconds from 200 seconds to 20 minutes, and 150 seconds for the rest of the simulation, are used for computing 3-D subsurface flow and is 5 seconds for computing 3-D subsurface transport, 2-D overland flow, and 2-D overland transport. An absolute error of 0.001 m is used to determine convergence for 3-D flow, while a relative error of 0.0001 is take as the stopping criterion for obtaining convergent solutions in 3-D transport, 2-D flow, and 2-D transport.

Figures 4.69 and 4.70 depict 2-D overland water depth and 3-D subsurface pressure head at various times. Figures 4.71 and 4.72 show the concentration distributions at time = 6 hours. By taking surface runoff into account (Figure 4.69), we do not observe unsaturated zone near the upper right corner (Figure 4.70), which is different from what we have obtained in Section 4.11 (Figure 4.64). Surface runoff also takes chemicals down to the right part of the system (Figure 4.71), and chemicals enter the subsurface through infiltration not only in $x \in [60 \text{ m}, 500 \text{ m}]$ but in $x \in [500 \text{ m}, 1000 \text{ m}]$ (Figure 4.72).

4.14. Example of 1-D/2-D/3-D flow

In this example, we consider a coupled 1-D/2-D/3-D flow system that is discretized as shown in Figure 4.73. Initially, ground surface is dry and the subsurface is assumed at a steady state that is determined by the following boundary conditions: no flux on the left ($x = 100$ m), the right ($x = 900$ m), and the bottom ($z = 0$ m) boundaries, a constant total head of 10 m for the lower part ($z \leq 10$ m) of both the front ($y = 0$ m) and the back ($y = 900$ m) boundaries; variable boundary condition of zero depth and zero rainfall for the surface on the top and for the rest of the front and the back boundary surfaces. The unsaturated soil

characteristics are described by Eqs. (4.25) and (4.26). The saturated conductivities are $K_{xx} = 10^{-4}$ m/s, $K_{yy} = 10^{-5}$ m/s, and $K_{zz} = 5 \times 10^{-6}$ m/s. The geometry and discretization of the 1-D/2-D surface system here is identical to that given in Section 4.8 and is not described again. The boundary conditions used for computing surface flow are the same as those employed in Section 4.8, except the water depth is forced to be zero at the upstream river/stream end (i.e., $x = 500$ m and $y = 900$ m) and on the top ridge of the overland domain (i.e., $x = 100$ m and $x = 900$ m). As the transient simulation begins, a rainfall of 10^{-5} m/s during the 1st hour and 1.5×10^{-5} m/s for the next 11 hours is applied to the system. An absolute error of 0.01 m is taken to determine 3-D flow convergence, and a relative error of 0.0001 is used to determine convergent solutions for both 1-D and 2-D flow. Variable time step sizes of 10 seconds from the beginning to 40 seconds, 40 seconds from 40 to 200 seconds, 100 seconds from 200 to 600 seconds, 150 seconds from 600 to 1200 seconds, 200 seconds from 1200 seconds to 1 hour, and 250 seconds from 1 hours to 12 hours are used for 3-D flow computation. A constant time step size of 2 seconds is used in calculating both 1-D and 2-D flow.

Figures 4.74 and 4.75 plot the water depth on 1-D and 2-D domains, respectively, at various times. Figures 4.76 and 4.77 depict the pressure head distribution and the Darcy velocity (specific discharge), respectively, on four vertical planes ($y = 100$ m, $y = 800$ m, $x = 500$ m, and $x = 800$ m) at various times. By matching Figures 4.74 through 4.76, we observe that the rainfall during the 1st hour is completely absorbed by ground soil, some water accumulates on ground surface and surface water flow exists at Time = 4 hours, and the entire surface domain, except for those boundary nodes at high locations (specified with zero depth boundary condition), is covered with water at the end of simulation (Time = 12 hours). Figure 4.77 gives us the idea how the Darcy velocity varies with time in this example. Basically, water movement is observed in the unsaturated zone (or the upper part) of the subsurface domain. It starts from surface/subsurface boundary due to infiltration. Its downward velocity increases with time first because the input of water from the top builds up head gradient in the unsaturated zone (from Time = 20 minutes to 4 hours), but decreases when the saturated zone expands and reduces head gradient subsequently (from Time = 4 hours to 12 hours).

4.15. Example of 1-D/2-D/3-D flow and transport

This example considers the most complicated situation that the model can handle: a coupled system of 1-D/2-D/3-D flow and transport. The domain geometry and flow condition here is identical to that in the previous section, except the saturated conductivity in the z-direction for 3-D subsurface flow is $K_{zz} = 2 \times 10^{-6}$ m/s. In chemical/sediment transport there are three dissolved chemicals ($\overline{C1}$, $\overline{C2}$, and $\overline{C3}$), one suspended and one bed sediments ($\overline{SS1}$ and $\overline{BS1}$), three particulate chemicals each on the suspended and the bed sediments ($\overline{PS1}$, $\overline{PS2}$, $\overline{PS3}$, and $\overline{PB1}$, $\overline{PB2}$, $\overline{PB3}$), one adsorbing site ($\overline{SITE1}$), and three adsorbed chemicals ($\overline{SORB1}$, $\overline{SORB2}$, and $\overline{SORB3}$). The sediment size is of cohesive type. The settling speed is 4.5×10^{-4} m/s. The critical shear stresses for deposition and erosion are 4.75 g/m^2 and 4.68 g/m^2 , respectively. The following reactions are taken into account.

$$\overline{C1} + \overline{C2} \rightleftharpoons \overline{C3} \quad k_f = 0.01, \quad k_b = 0.005 \quad (4.29)$$

$$\overline{C1} + \overline{SS1} \rightleftharpoons \overline{PS1} + \overline{SS1} \quad k_f = 0.0001, \quad k_b = 0.0 \quad (4.30)$$

$$\overline{C2} + \overline{SS1} \rightleftharpoons \overline{PS2} + \overline{SS1} \quad k_f = 0.0001, \quad k_b = 0.0 \quad (4.31)$$

$$\overline{C3} + \overline{SS1} = \overline{PS3} + \overline{SS1} \quad k_f = 0.0001, \quad k_b = 0.0 \quad (4.32)$$

$$\overline{C1} + \overline{BS1} = \overline{PB1} + \overline{BS1} \quad k_f = 0.00001, \quad k_b = 0.0 \quad (4.33)$$

$$\overline{C2} + \overline{BS1} = \overline{PB2} + \overline{BS1} \quad k_f = 0.00001, \quad k_b = 0.0 \quad (4.34)$$

$$\overline{C3} + \overline{BS1} = \overline{PB3} + \overline{BS1} \quad k_f = 0.00001, \quad k_b = 0.0 \quad (4.35)$$

$$\overline{C1} + \overline{SITE1} = \overline{SORB1} \quad k_f = 0.001, \quad k_b = 0.0002 \quad (4.36)$$

$$\overline{C2} + \overline{SITE1} = \overline{SORB2} \quad k_f = 0.001, \quad k_b = 0.0001 \quad (4.37)$$

$$\overline{C3} + \overline{SITE1} = \overline{SORB3} \quad k_f = 0.001, \quad k_b = 0.0 \quad (4.38)$$

Initially, only do bed sediments and adsorbing sites exist in the system. The initial concentrations are 10 g/m³ for the bed sediment on overland, 100 g/m³ for the bed sediment in river/stream, and 2 g/m³ for the adsorbing site. As the transient simulation starts, $\overline{C1}$, $\overline{C2}$, and $\overline{C3}$ of 1 g/m³ come into the system through rainfall and this is the only source that chemicals would enter the system. To achieve the transient simulation associated with such a condition, we employ surface/subsurface variable boundary conditions for the top boundary and a variable boundary condition with a zero incoming concentration for the front (y = 0 m) and back (y = 900 m) subsurface boundaries. In addition, we apply the no-flux condition for the right (x = 900 m), the left (x = 100 m), and the bottom (z = 0 m) boundaries (Figure 4.73). A relative error of 10⁻⁴ is used to determine convergence in transport computations. The longitudinal dispersivity is 0.1 m, the transverse dispersivity is 0.01 m, and the diffusion coefficient is 10⁻⁵ m²/s. Time step sizes for 3-D flow is the same as those in the previous section, but 10 seconds and 2.5 seconds are used for 2-D and 1-D simulations, respectively.

Figures 4.78 through 4.80 show the numerical results of river/stream water depth, overland water depth, and subsurface pressure head at various times of the 12 hour simulation. Figures 4.81 through 4.83 plot the concentration distribution of dissolved chemicals in 1-D, 2-D, and 3-D domains, respectively, at the end of simulation. Figures 4.84 and 4.85 plot the sediment concentrations in 1-D and 2-D systems, respectively. Figures 4.86 and 4.87 depict the first particulate chemicals on sediments in 1-D and 2-D systems, respectively. Figures 4.88 shows the concentration of the adsorbing site and adsorbed chemicals in the 3-D subsurface domain.

With a smaller K_{zz} in the subsurface, we observe more water on surface in this example than that in the previous one (i.e., in Section 4.14). Because the water depth is set to be zero on the upstream boundary of both overland and river/stream systems, we always define zero concentration associated with those boundary nodes (Figures 4.81, 4.82, 4.86, and 4.87). We observe the removal of bed sediment in river/stream (Figure 4.84) but do not have change of sediment distribution on overland (Figure 4.85). This can also be verified by matching Figure 4.84 with Figure 4.86 and Figure 4.85 with Figure 4.87. In this example, infiltration exists on the surface/subsurface interface through the entire simulation. Therefore, the incoming variable boundary condition is used to account for the top boundary in dealing with 3-D subsurface transport. Because of this and because the chemistry in the surface system is the same for $\overline{C1}$ and $\overline{C2}$ (Eqs. (4.29), (4.30), (4.31), (4.33), and (4.34)), we obtain identical concentration distribution for these two dissolved

chemicals (Figures 4.81 and 4.82). However, their concentration distributions are not same in the subsurface (Figure 4.83) because they are involved in adsorption reactions with different backward rate constants (Eqs. (4.36) and (4.37)). Among the adsorbed chemicals, $\overline{\text{SORB3}}$ has the highest maximum concentration while $\overline{\text{SORB1}}$ has the lowest maximum concentration (Figure 4.88). This is mainly because the backward reaction rate constant associated with $\overline{\text{SORB3}}$ is the smallest ($k_b = 0$) and that associated with $\overline{\text{SORB1}}$ is the largest ($K_b = 0.0002$) among the three adsorption reactions.

Section 5. SUMMARY AND CONTINUING WORK

A numerical model has been developed to simulate water flow and sediment and reactive chemical transport in watershed systems. The mathematical basis and numerical approaches of the model was given in Sections 2 and 3. Section 4 has demonstrated that the model was able to deal with various configurations of problems involving flow and sediment and chemical transport over watersheds with a wide range of ground surface slopes. Fifteen example problems were presented to illustrate the basic capability of the model.

Much experience has been gained throughout the research of this project. It was demonstrated that the method of characteristics can provide accurate numerical simulations in solving the dynamic wave model when slopes of the ground surface are small. However, its application to solving problems with steep slopes has proved elusive. On the other hand, the Lagrangian approach was illustrated to be robust in solving diffusion and kinematic wave models. However, kinematic and diffusion wave models can yield accurate solutions only for cases of mild to steep slope problems. For cases of problems involving small slopes, the kinematic/diffusion wave models could not generate accurate results, even though the models can be solved easily. The kinematic wave model cannot address the effects of backwater on flow dynamics over watersheds. In consideration of robustness (i.e., easy to solve with numerical methods) and accuracies, a hybrid model of adaptively choosing appropriate models (kinematic, diffusion, or dynamic wave models) for different regions of a watershed is desirable.

Using the predictor-corrector approach to solving the transport equations, we have made the computation effective and robust. For each time, we need to solve the advection/dispersion transport only one time in the predictor step, and the chemical reaction system can be solved node by node in the corrector step. The reaction chemistry can be quite general. All reactions whose rates can be described by the collision theory are included in the model.

To improve the model, the following work is recommended.

1. Developing a hybrid flow scheme where the dynamic, diffusion, and kinematic wave models are applied to different parts of the surface system adaptively based on a criterion that is to be established.
2. Incorporating density effects.
3. Incorporating chemical equilibrium.
4. Modeling the existence of interstitial water associated with bed sediments.

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Backward tracking along characteristics for 1-D channel flow

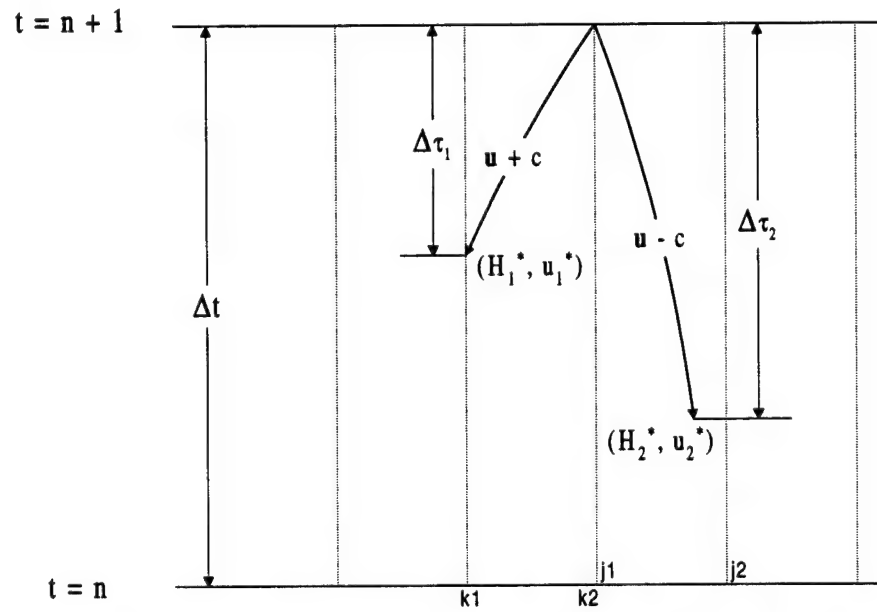


Figure 3.1. Tracking along characteristics in solving 1-D dynamic wave equation.

Backward tracking along characteristics for 2-D overland flow

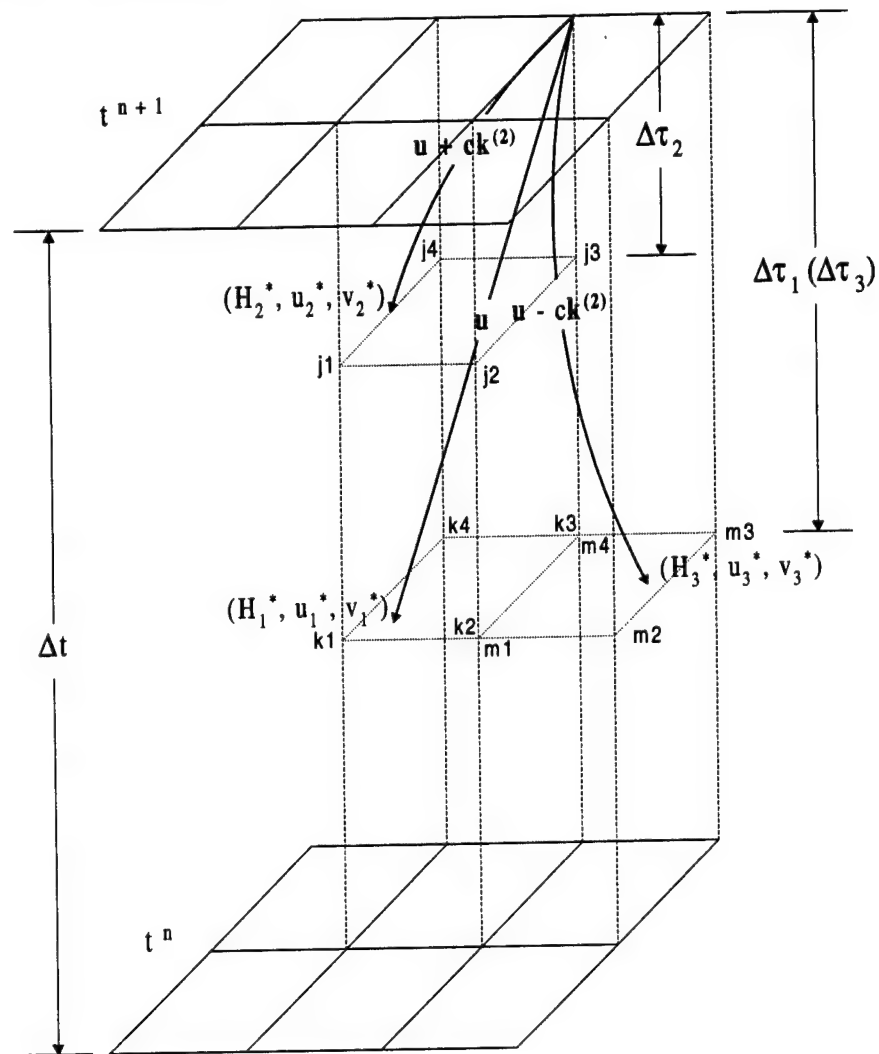


Figure 3.2. Tracking along characteristics in solving 2-D dynamic wave equation.

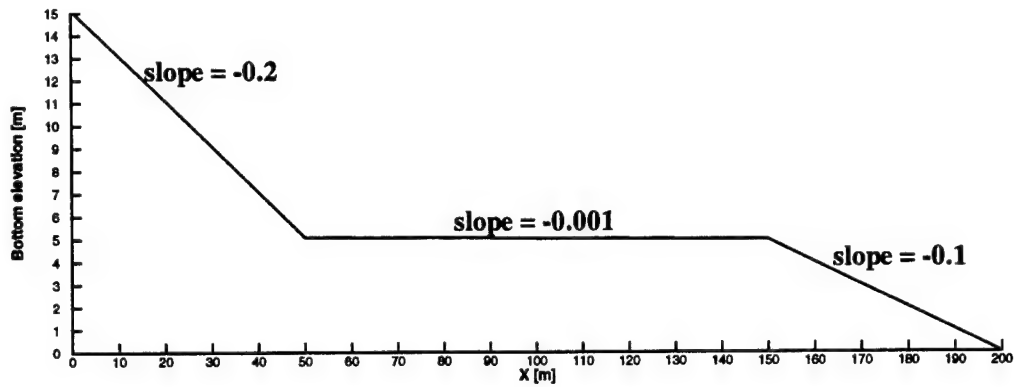


Figure 4.1. The bottom elevation of Example 1 of 1-D river/stream flow.

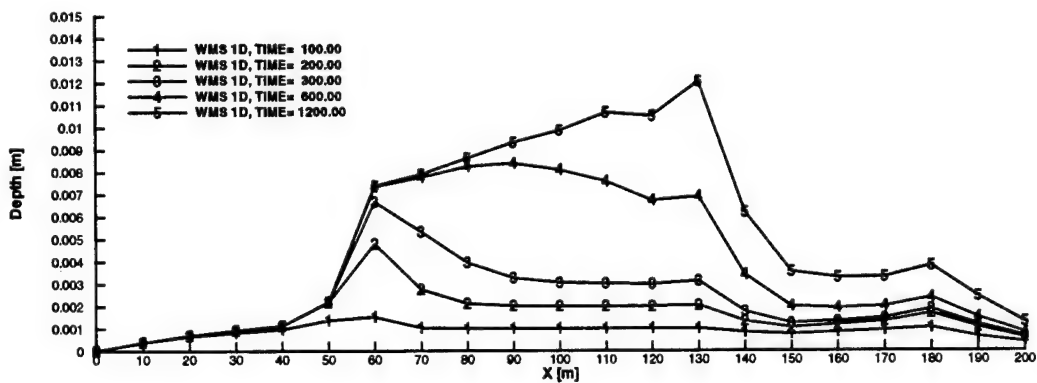


Figure 4.2. Water depth at various times for Example 1 of 1-D river/stream flow.

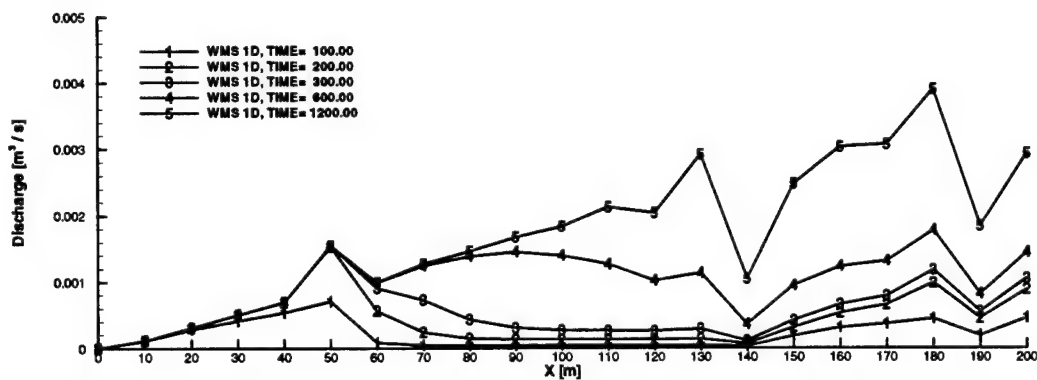


Figure 4.3. Discharge at various times for Example 1 of 1-D river/stream flow.

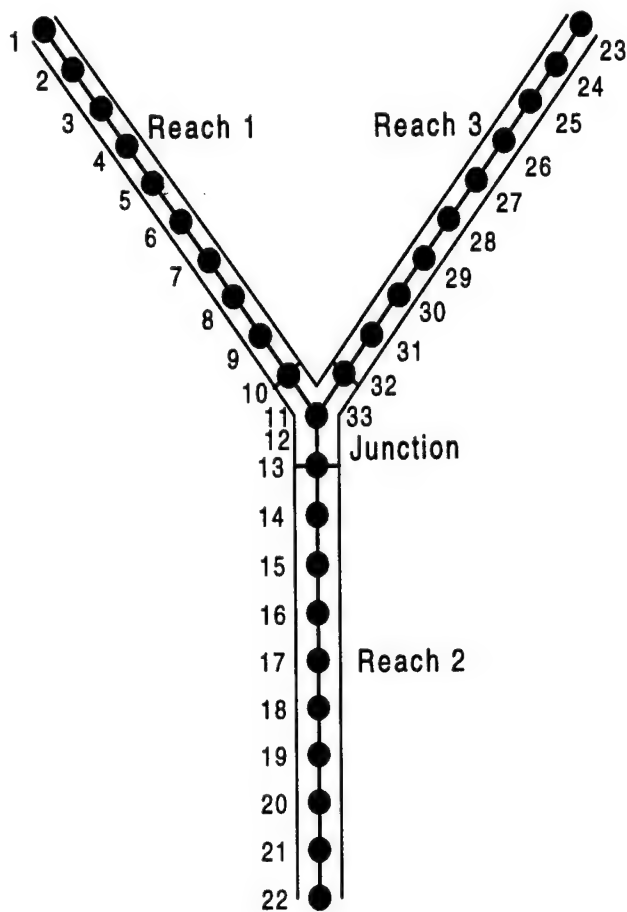


Figure 4.4. River/stream network for Example 2 of 1-D river/stream flow.

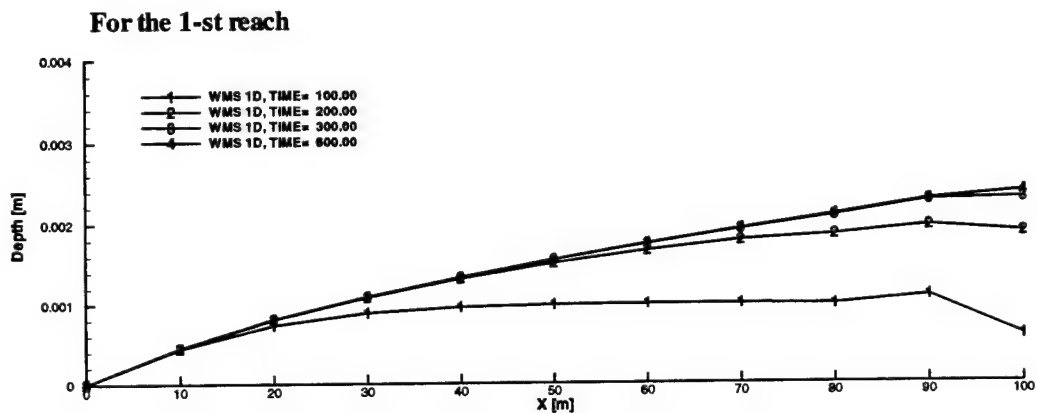


Figure 4.5. Water depth of Reach 1 at various times for Example 2 of 1-D river/stream flow.

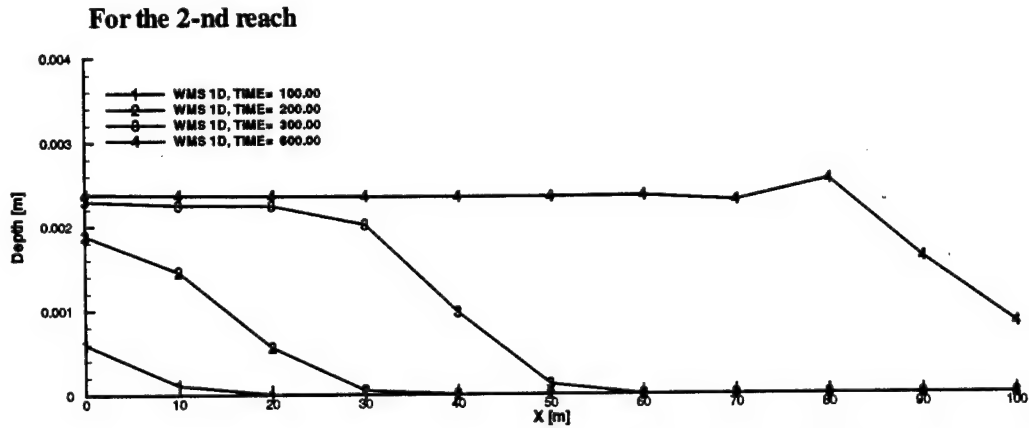


Figure 4.6. Water depth of Reach 2 at various times for Example 2 of 1-D river/stream flow.

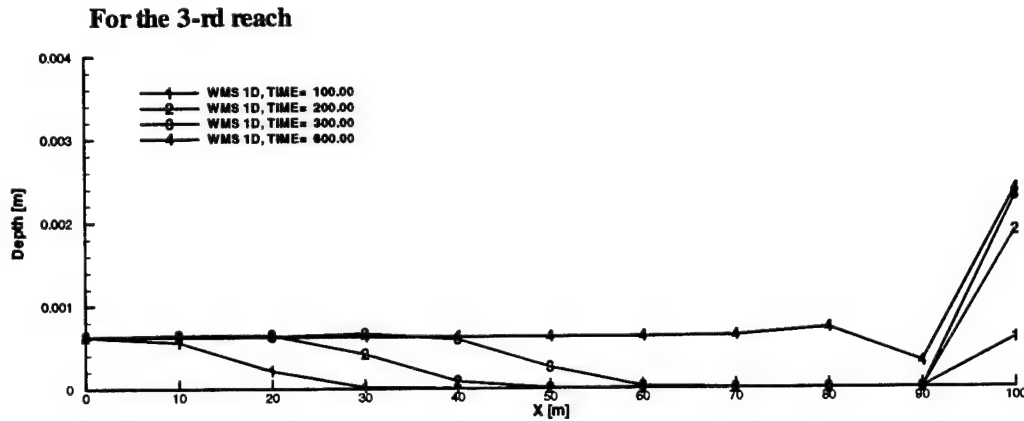


Figure 4.7. Water depth of Reach 3 at various times for Example 2 of 1-D river/stream flow.

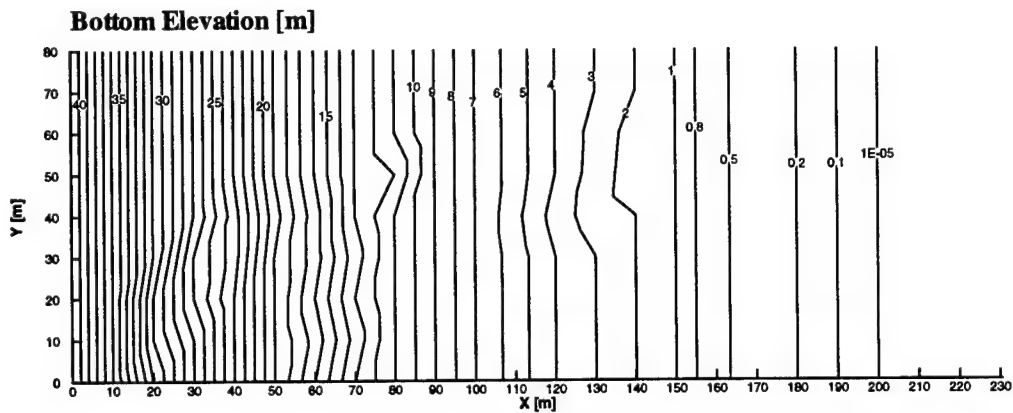


Figure 4.8. The contour of bottom elevation for Example 1 of 2-D overland flow.

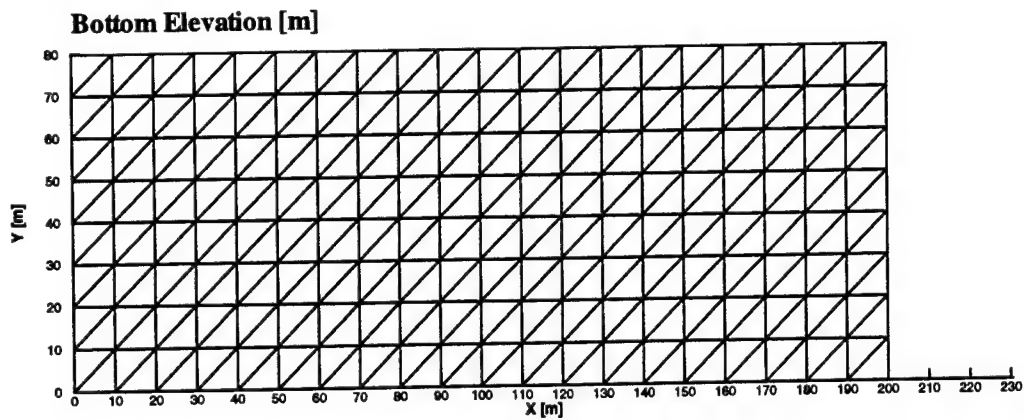


Figure 4.9. Discretization for Example 1 of 2-D overland flow.

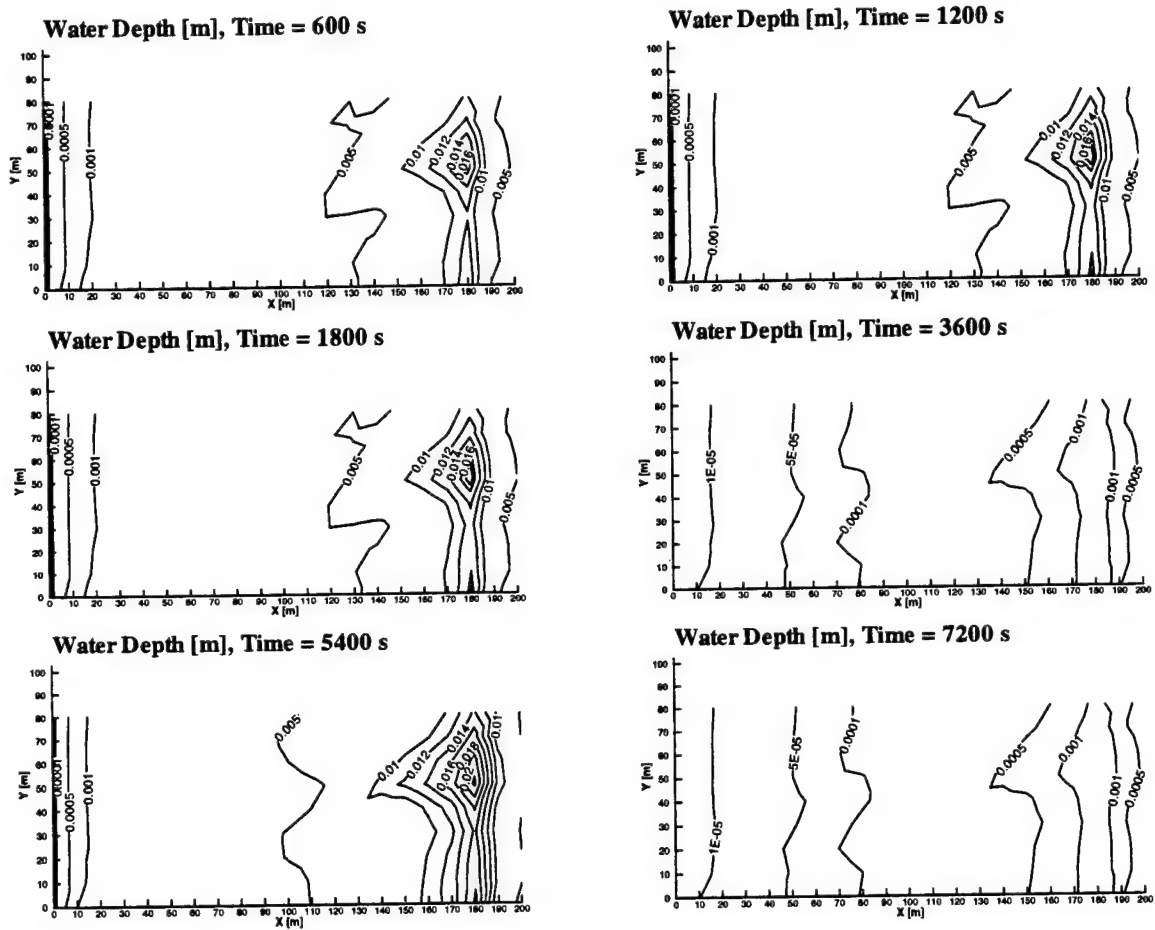
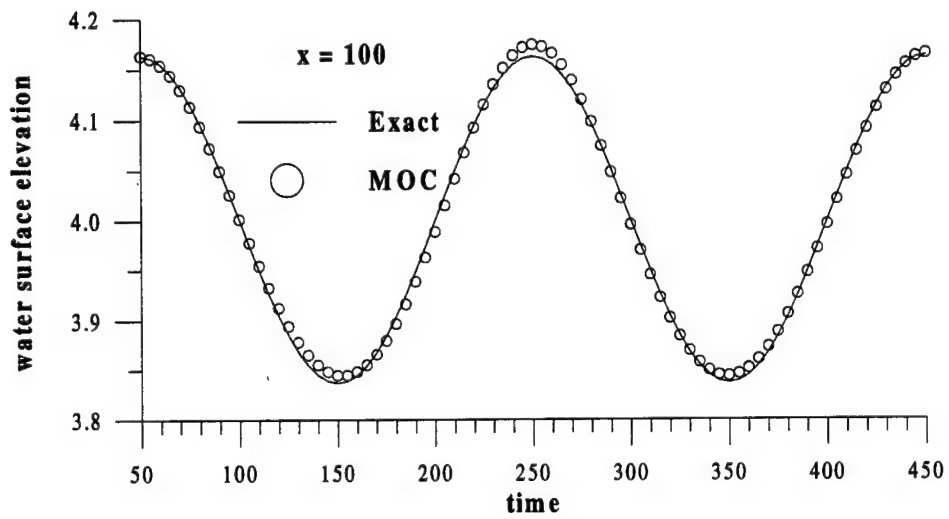


Figure 4.10. Water depth at various times for Example 1 of 2-D overland flow.

(a)



(b)

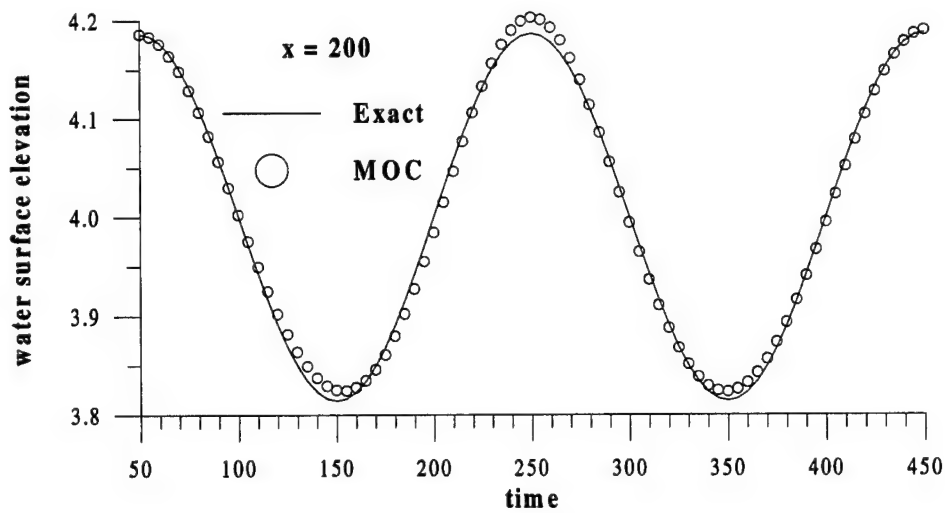


Figure 4.11. Comparison of water depth between analytical solutions and numerical results for Example 2 of 2-D overland flow.

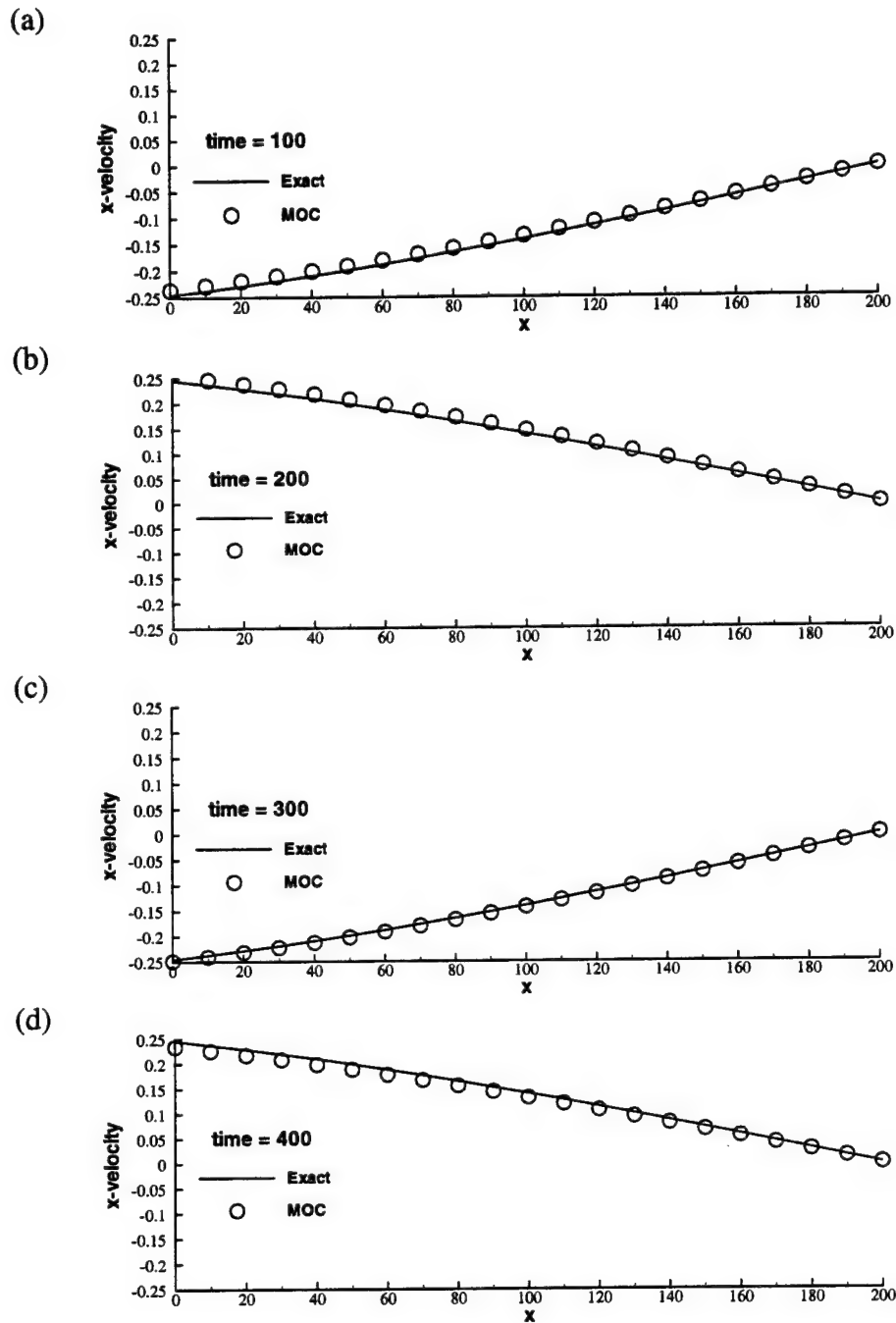
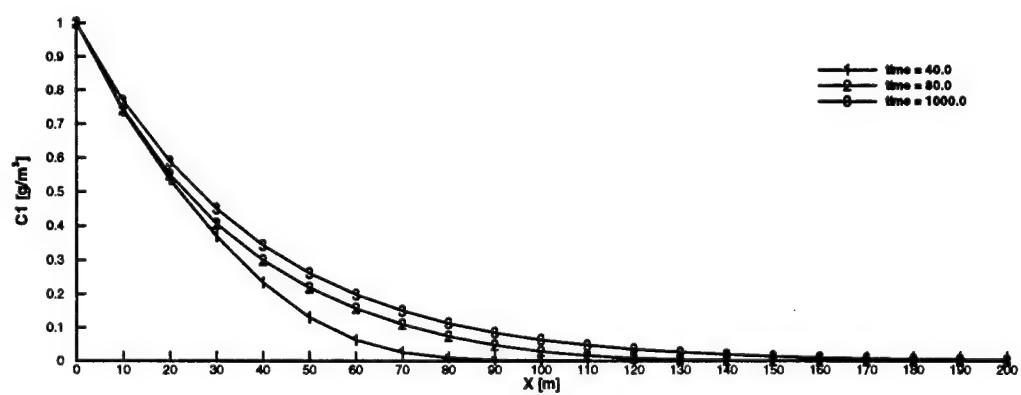
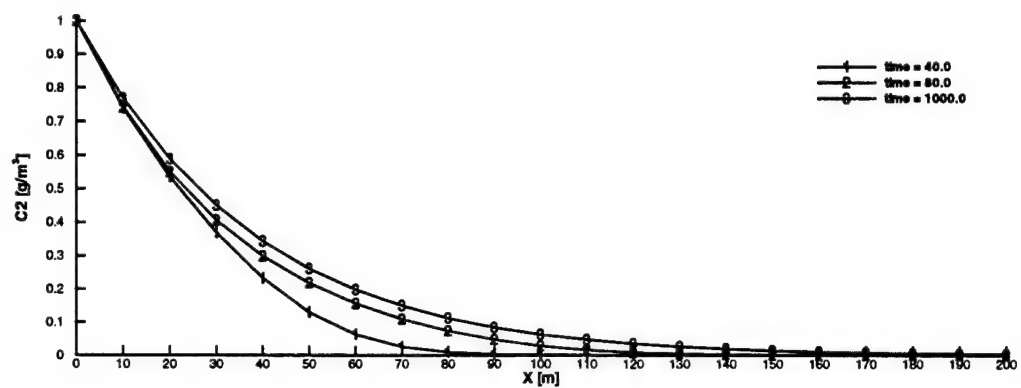


Figure 4.12. Comparison of velocity between analytical solutions and numerical results for Example 2 of 2-D overland flow.

(a)



(b)



(c)

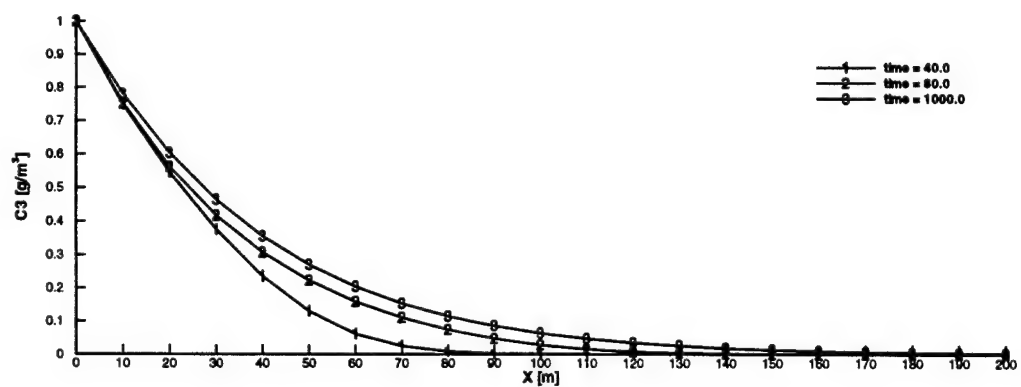
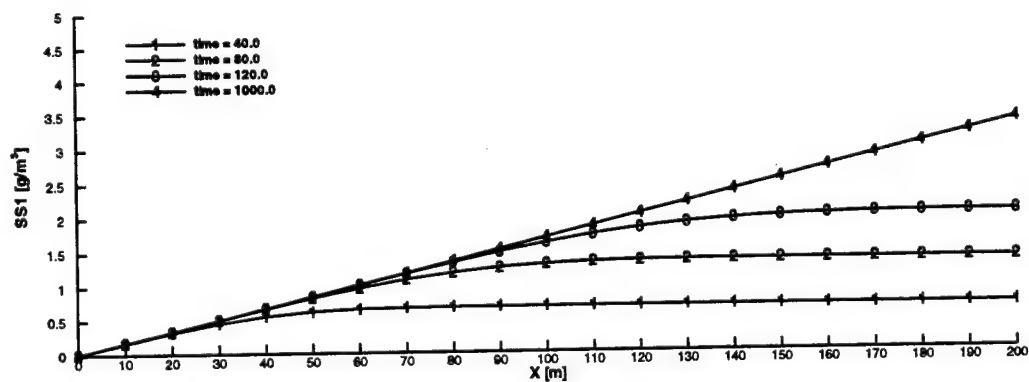
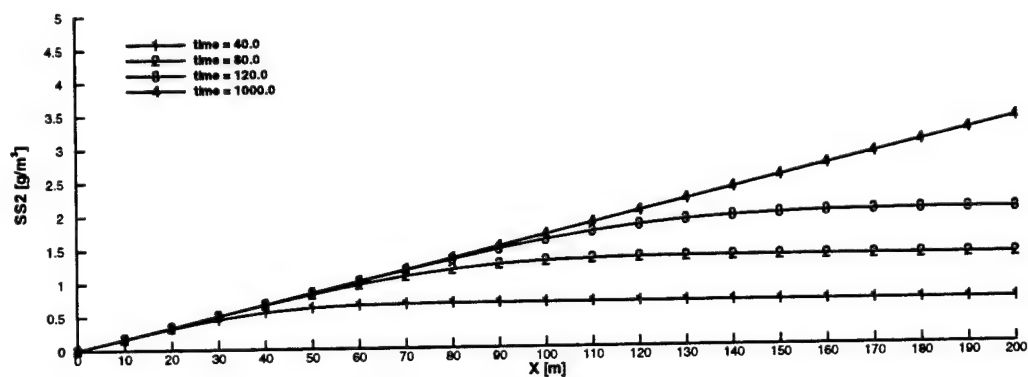


Figure 4.13. Concentrations of the (a) the first, (b) the second, and (c) the third dissolved chemicals for the example of 1-D river/stream transport.

(a)



(b)



(c)

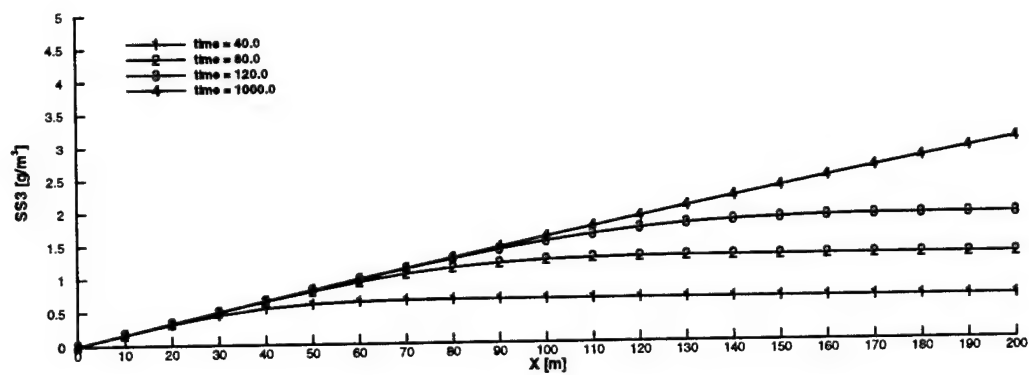
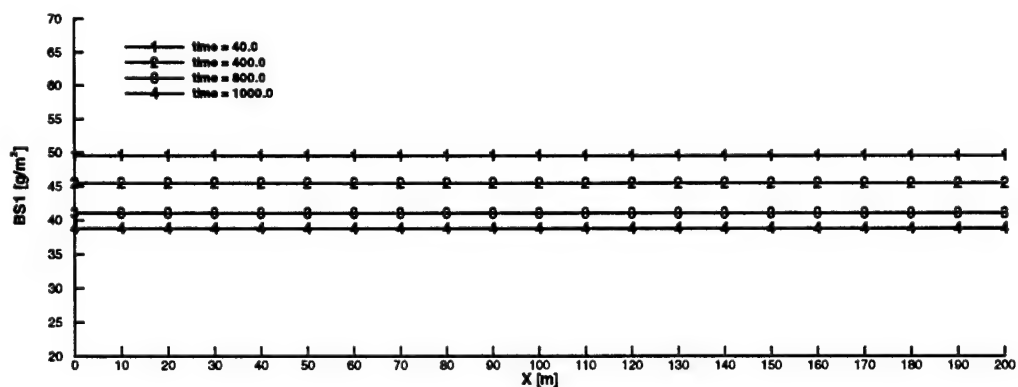
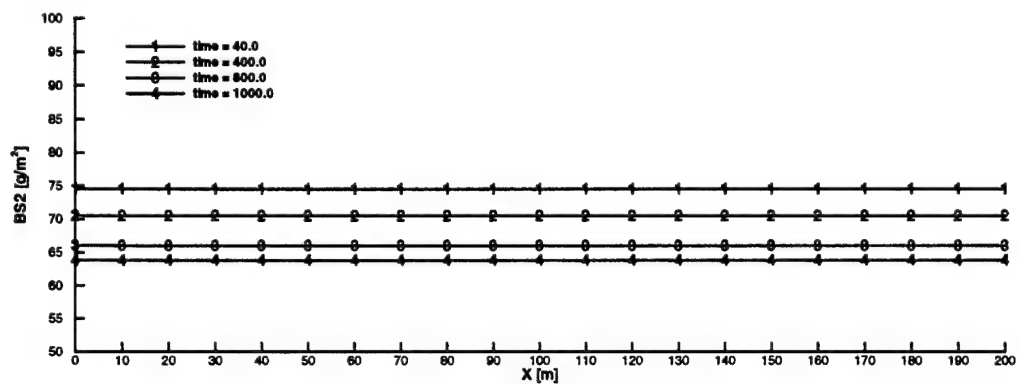


Figure 4.14. Concentrations of (a) the first, (b) the second, and (c) the third suspended sediments for the example of 1-D river/stream transport.

(a)



(b)



(c)

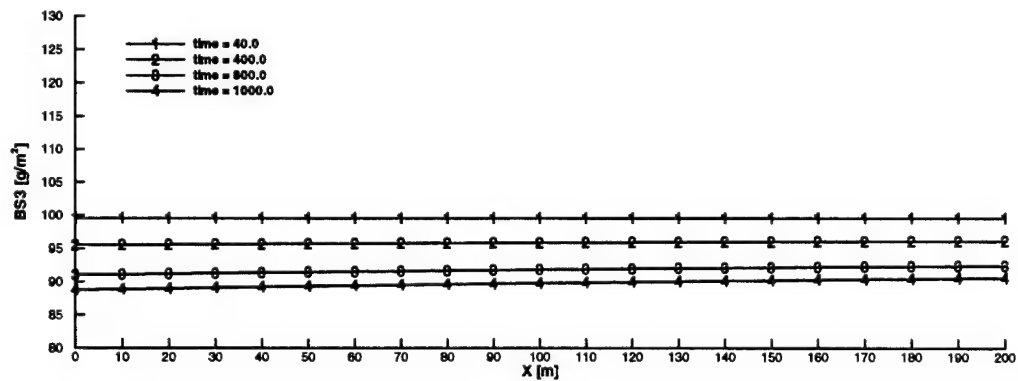
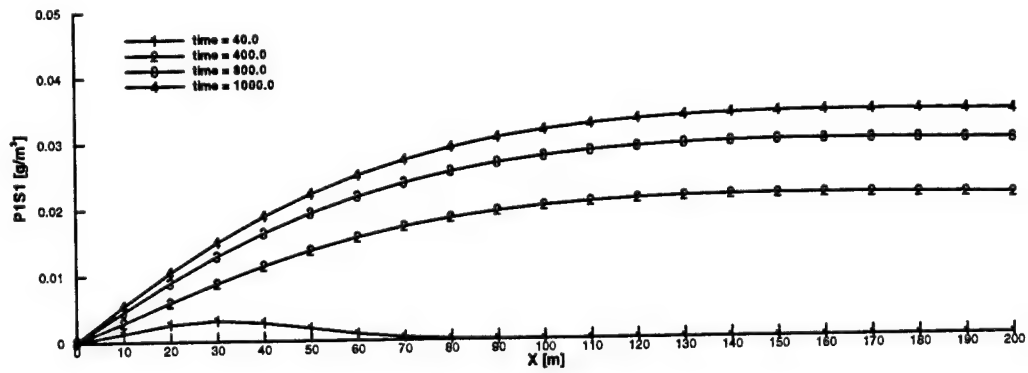
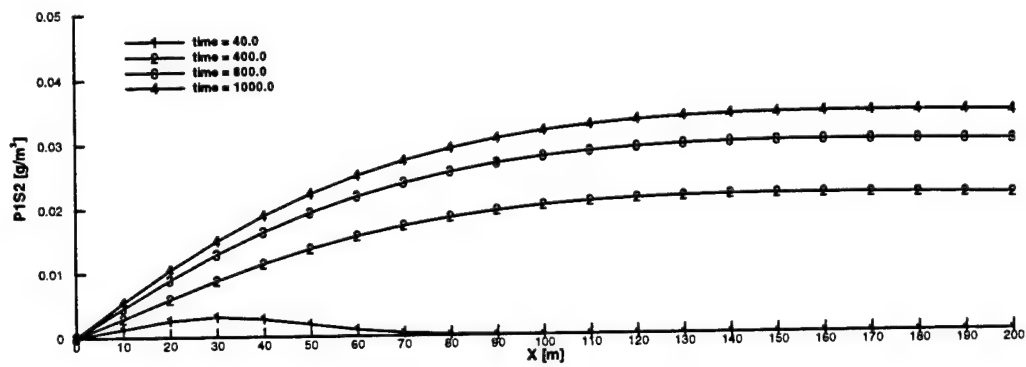


Figure 4.15. Concentrations of (a) the first, (b) the second, and (c) the third bed sediments for the example of 1-D river/stream transport.

(a)



(b)



(c)

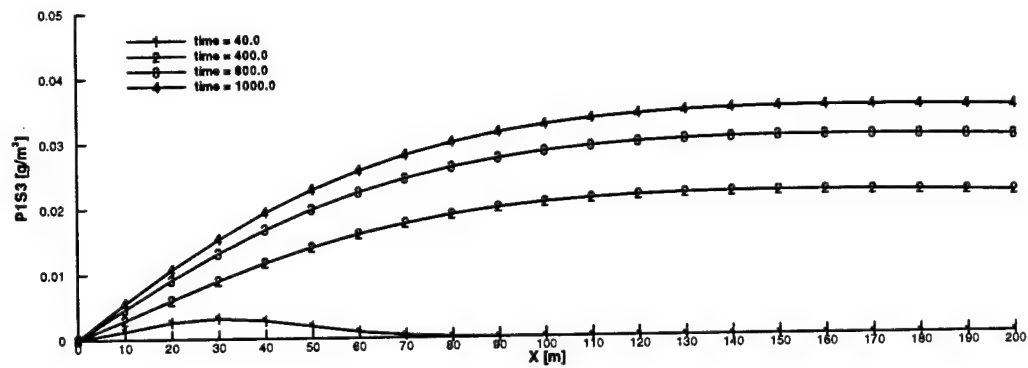
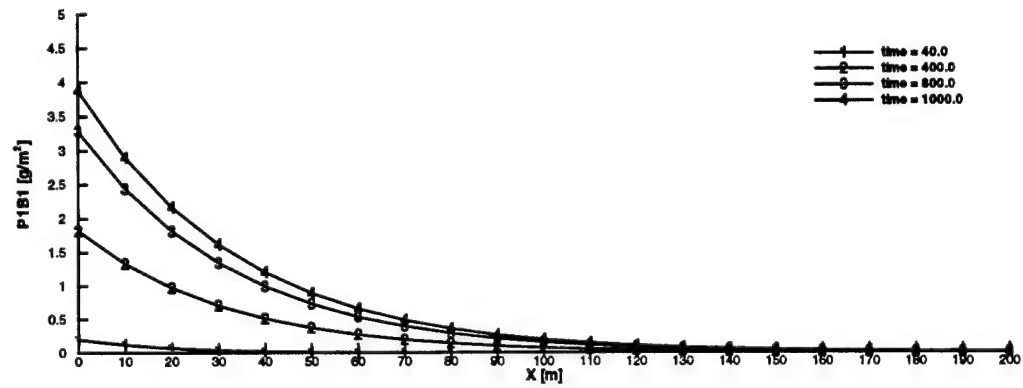
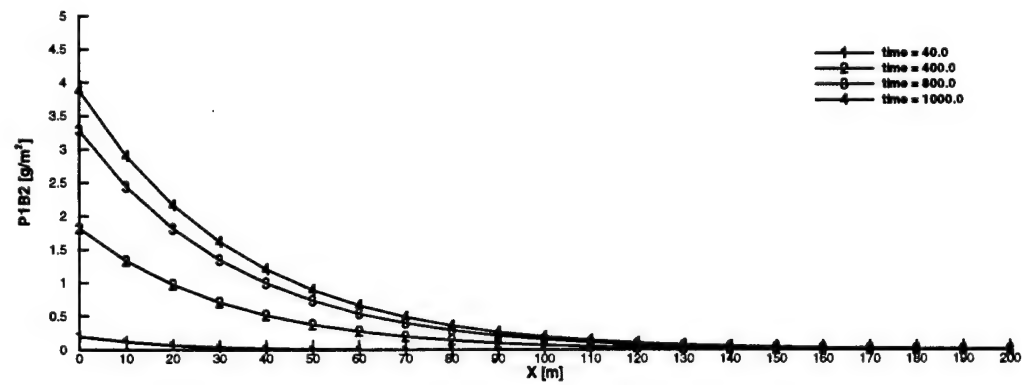


Figure 4.16. Concentrations of the first particulate chemical on (a) the first, (b) the second, and (c) the third suspended sediments for the example of 1-D river/stream transport.

(a)



(b)



(c)

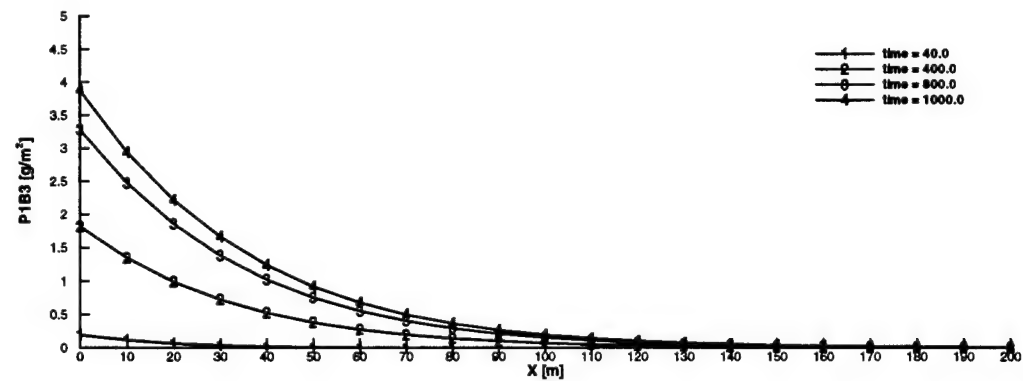


Figure 4.17. Concentrations of the first particulate chemical on (a) the first, (b) the second, and (c) the third bed sediments for the example of 1-D river/stream transport.

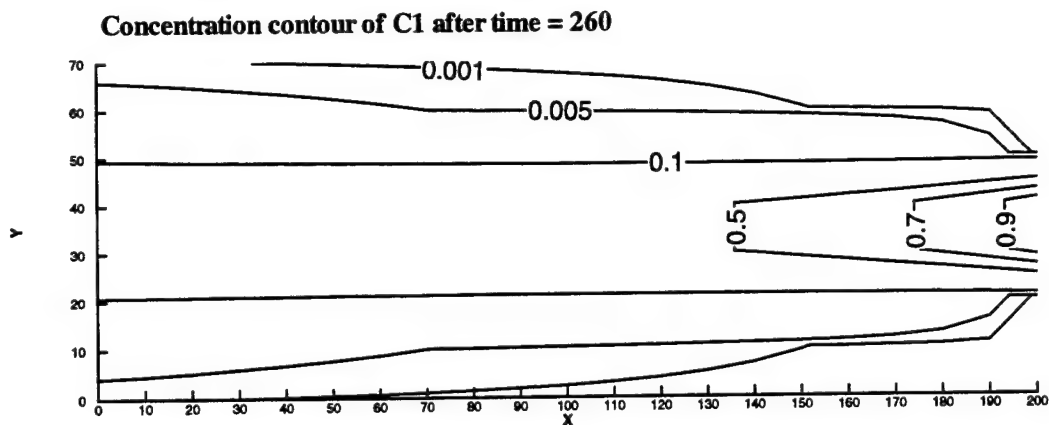


Figure 4.18. Concentration contour of the first dissolved chemical at time = 260 s for the example of 2-D overland transport.

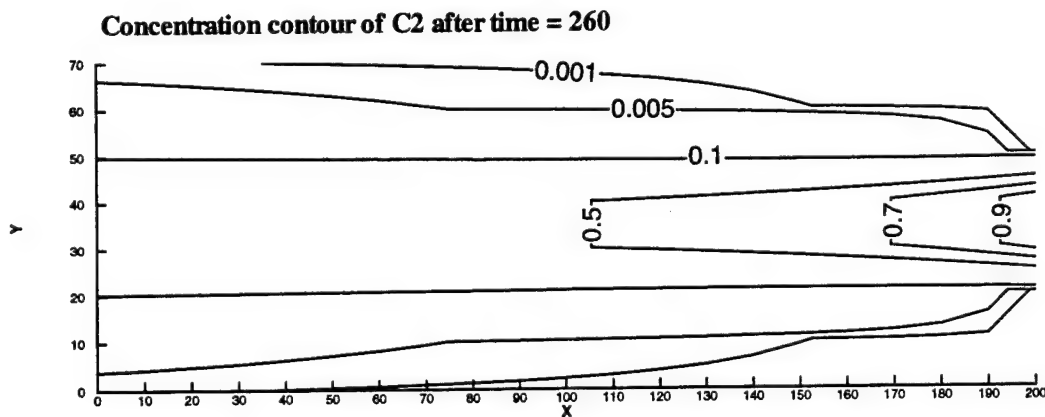


Figure 4.19. Concentration contour of the second dissolved chemical at time = 260 s for the example of 2-D overland transport.

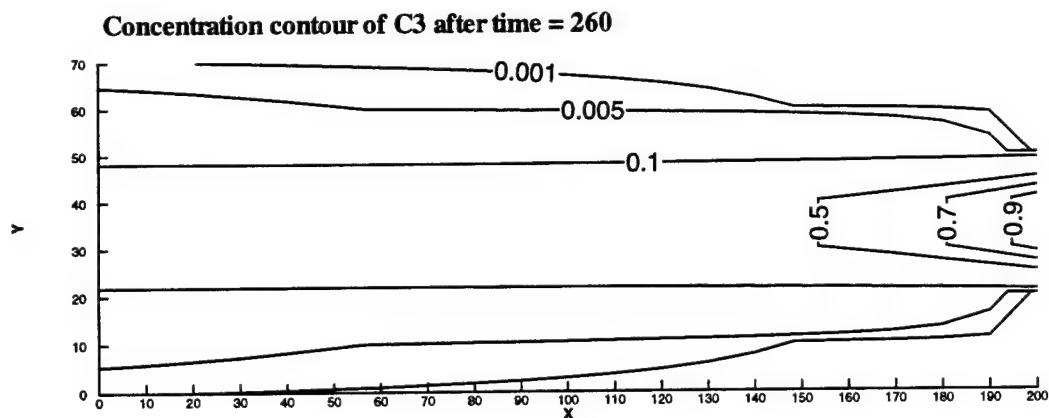


Figure 4.20. Concentration contour of the third dissolved chemical at time = 260 s for the example of 2-D overland transport.

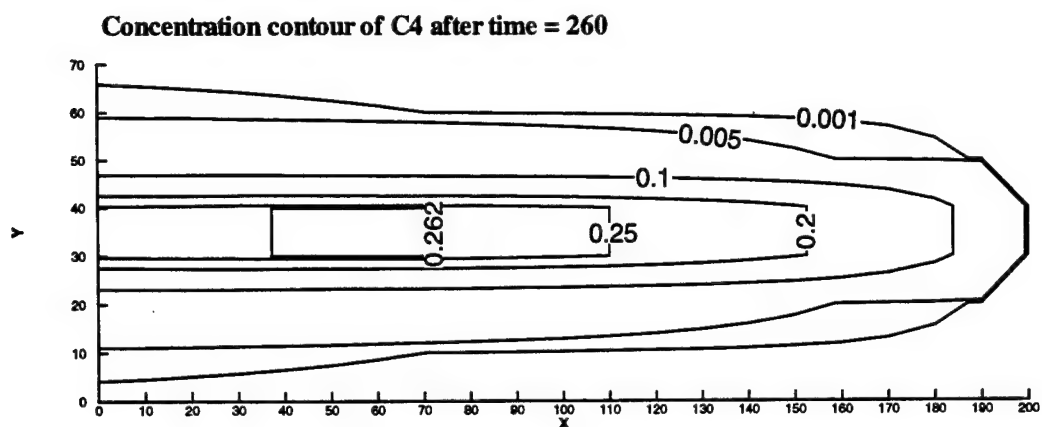


Figure 4.21. Concentration contour of the fourth dissolved chemical at time = 260 s for the example of 2-D overland transport.

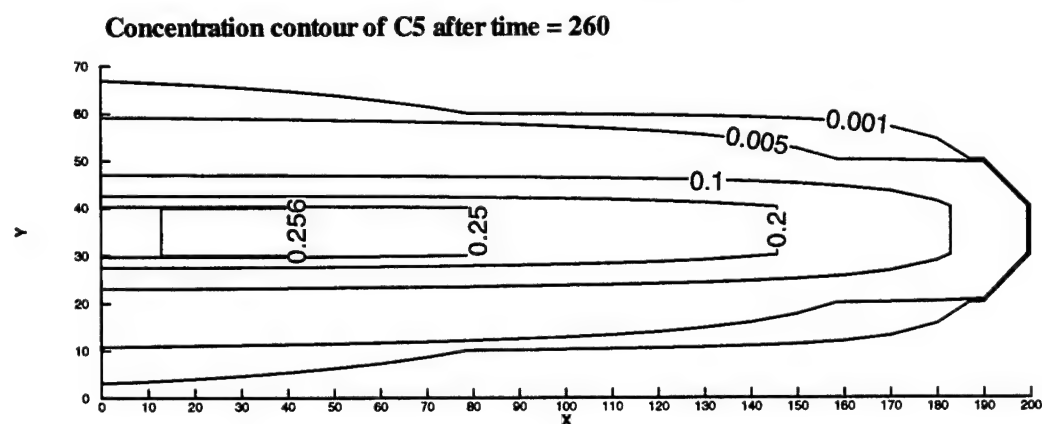


Figure 4.22. Concentration contour of the fifth dissolved chemical at time = 260 s for the example of 2-D overland transport.

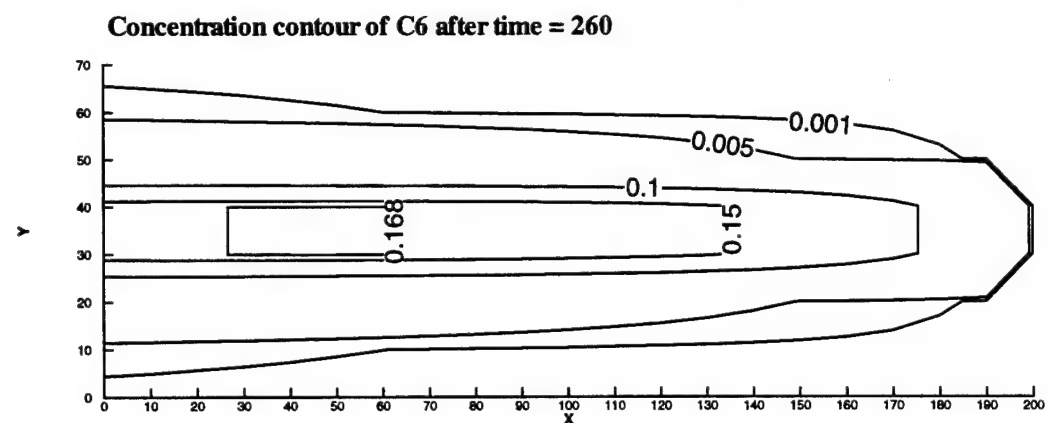


Figure 4.23. Concentration contour of the sixth dissolved chemical at time = 260 s for the example of 2-D overland transport.

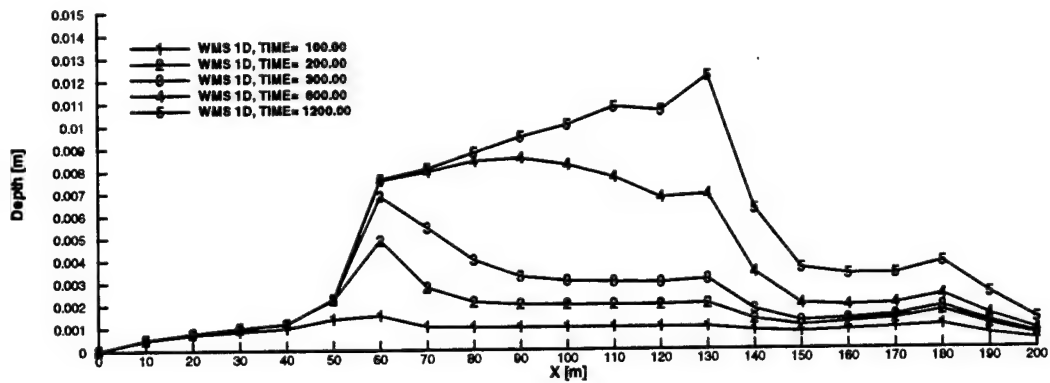


Figure 4.24. Water depth at various times for the example of 1-D river/stream flow and transport.

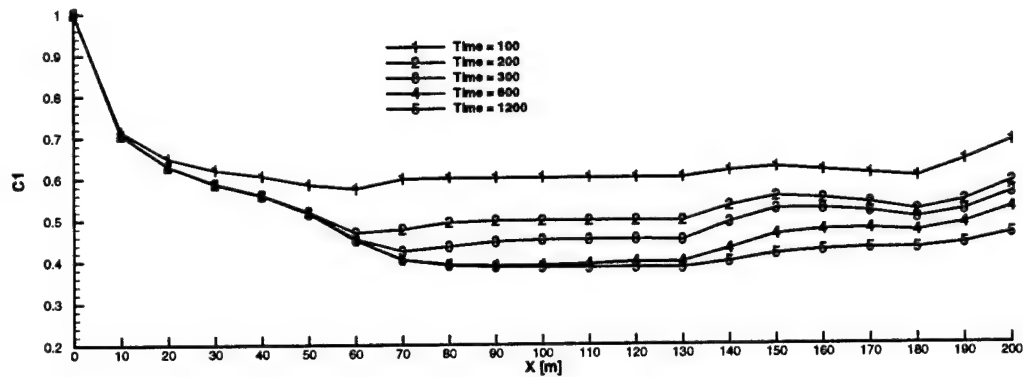


Figure 4.25. Concentration of the first dissolved chemical at various times for the example of 1-D river/stream flow and transport.

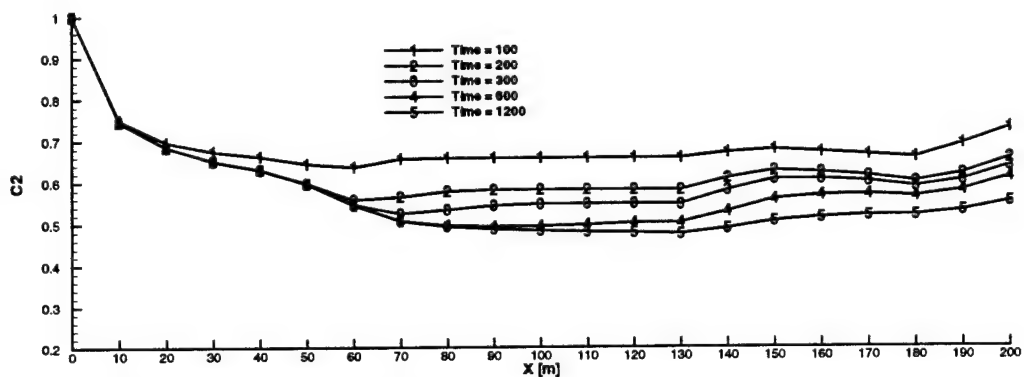


Figure 4.26. Concentration of the second dissolved chemical at various times for the example of 1-D river/stream flow and transport.

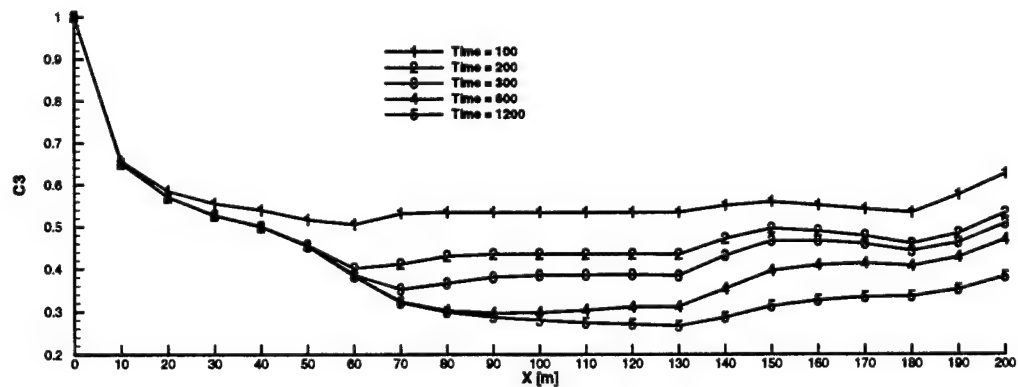


Figure 4.27. Concentration of the third dissolved chemical at various times for the example of 1-D river/stream flow and transport.

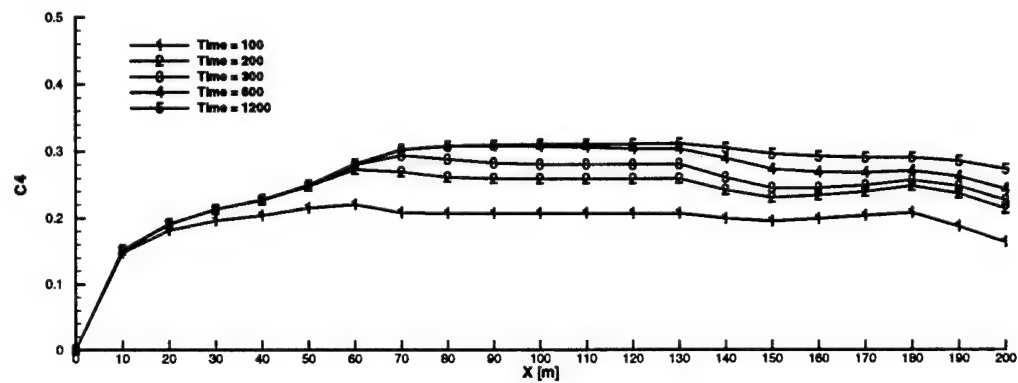


Figure 4.28. Concentration of the fourth dissolved chemical at various times for the example of 1-D river/stream flow and transport.

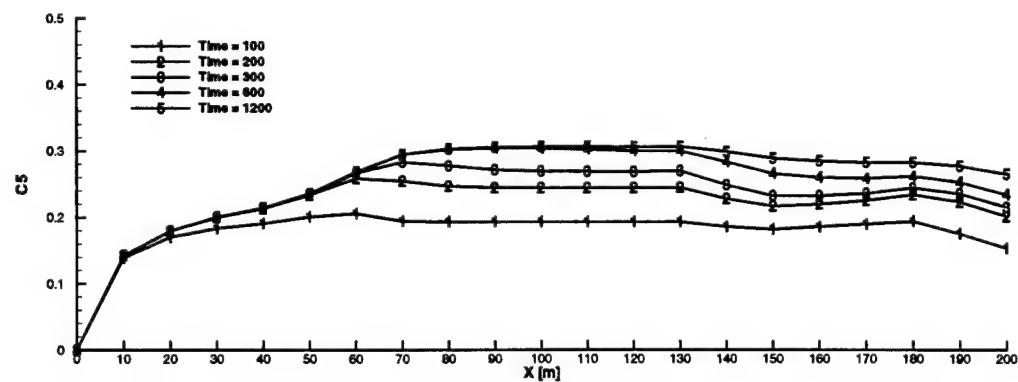


Figure 4.29. Concentration of the fifth dissolved chemical at various times for the example of 1-D river/stream flow and transport.

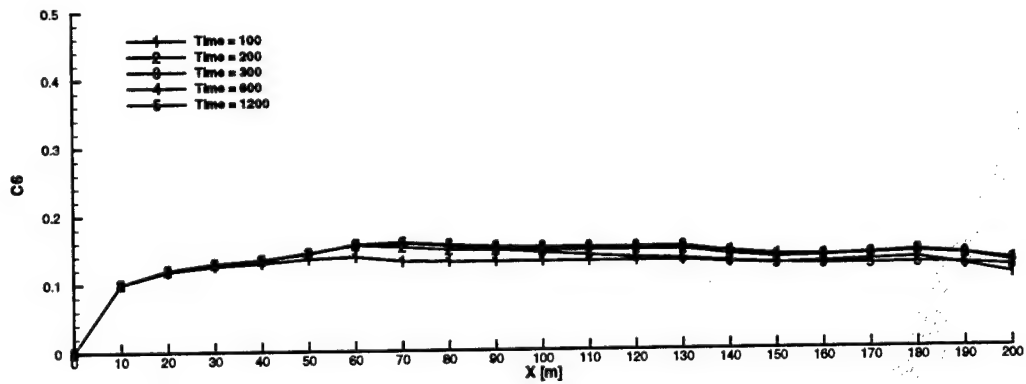


Figure 4.30. Concentration of the sixth dissolved chemical at various times for the example of 1-D river/stream flow and transport.

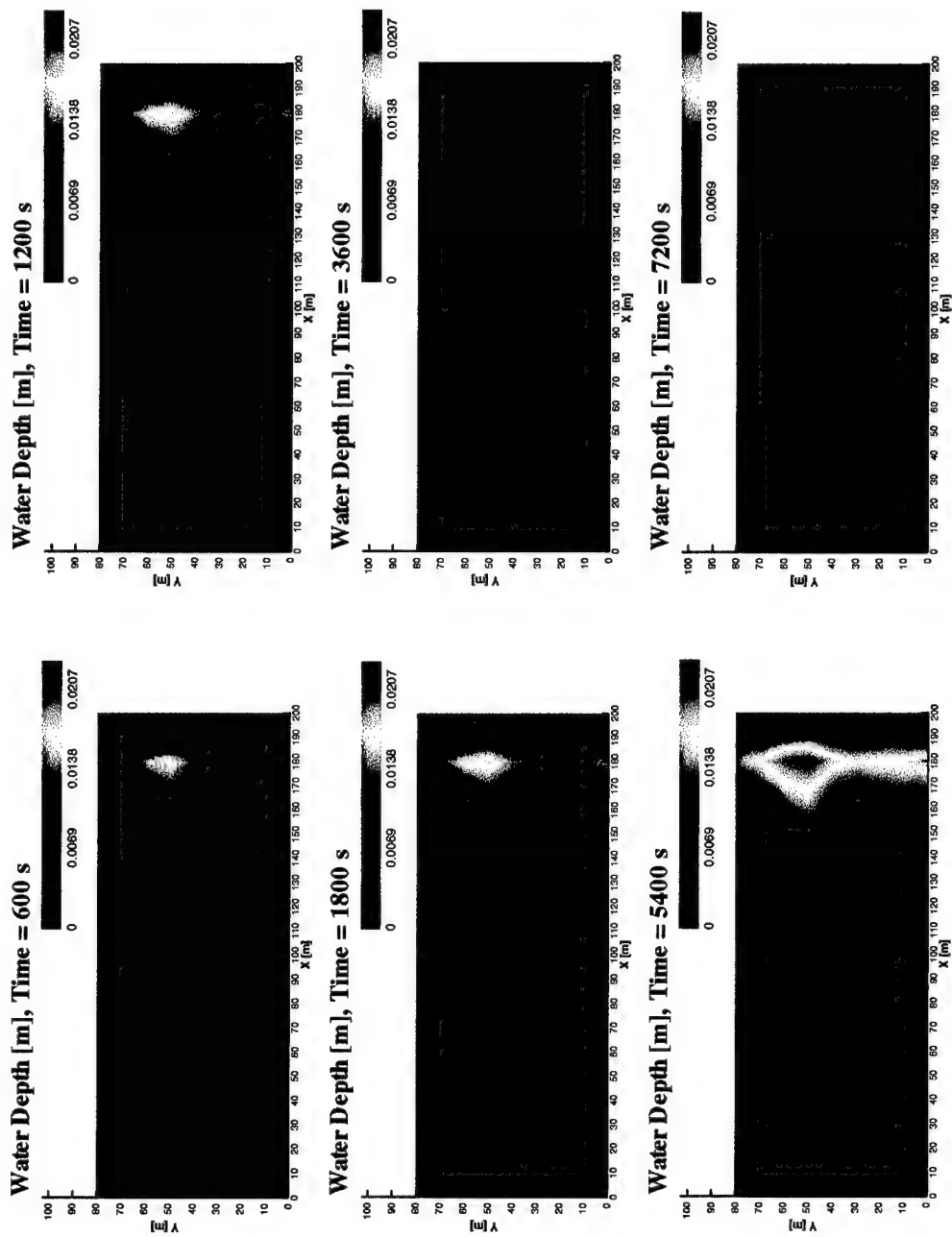


Figure 4.31. Water depth at various times for the example of 2-D overland flow and transport.

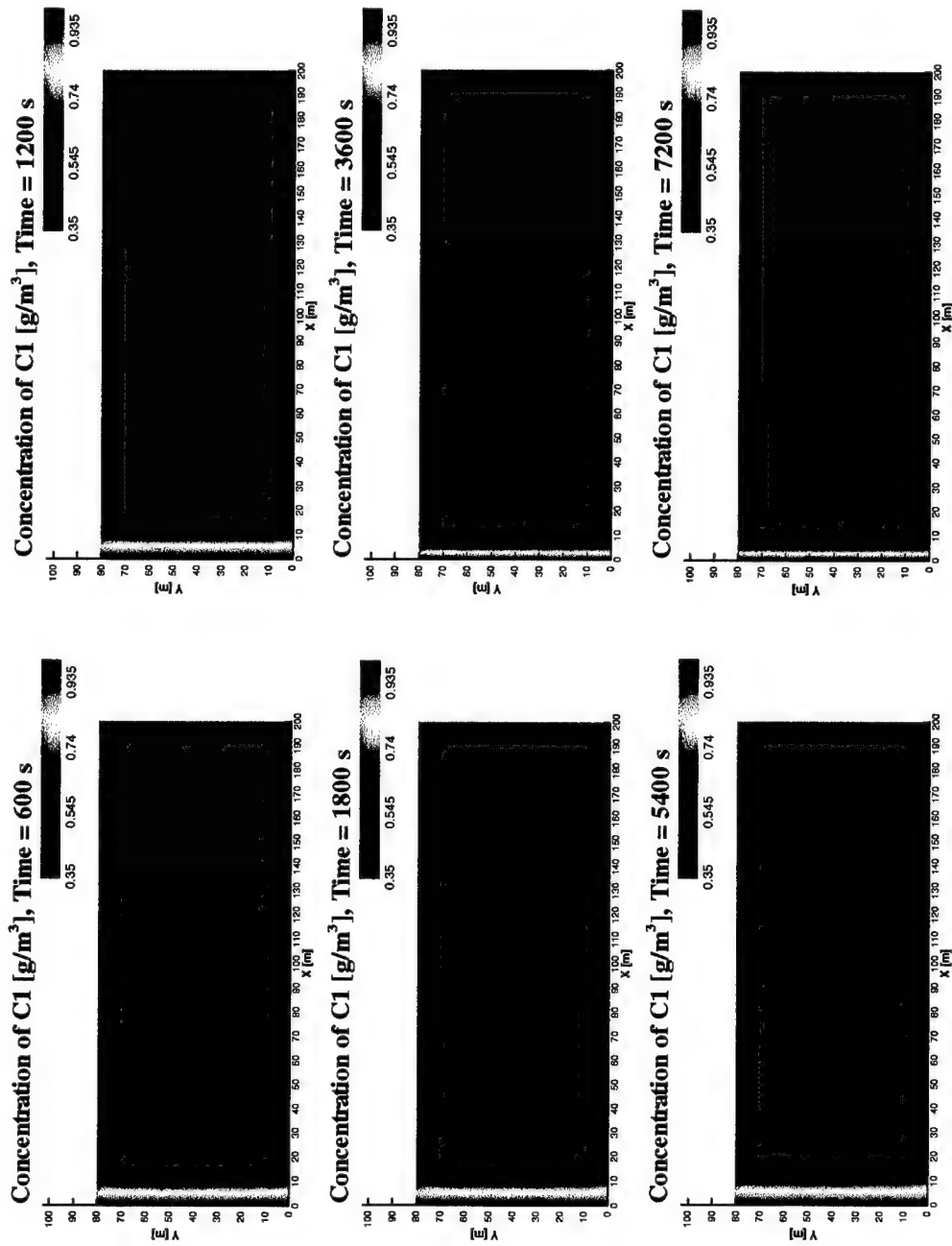


Figure 4.32. Concentration of the first dissolved chemical at various times for the example of 2-D overland flow and transport.

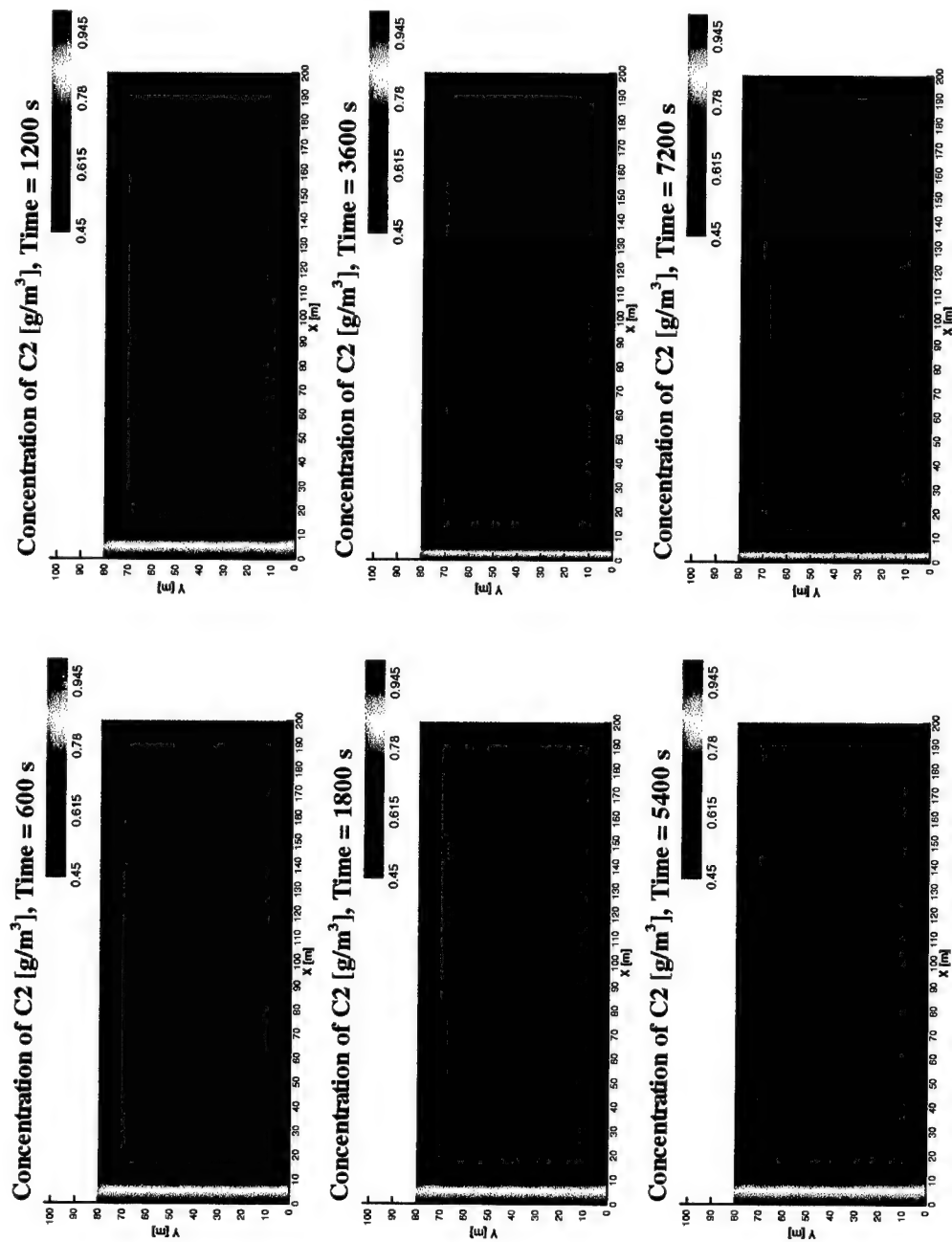


Figure 4.33. Concentration of the second dissolved chemical at various times for the example of 2-D overland flow and transport.

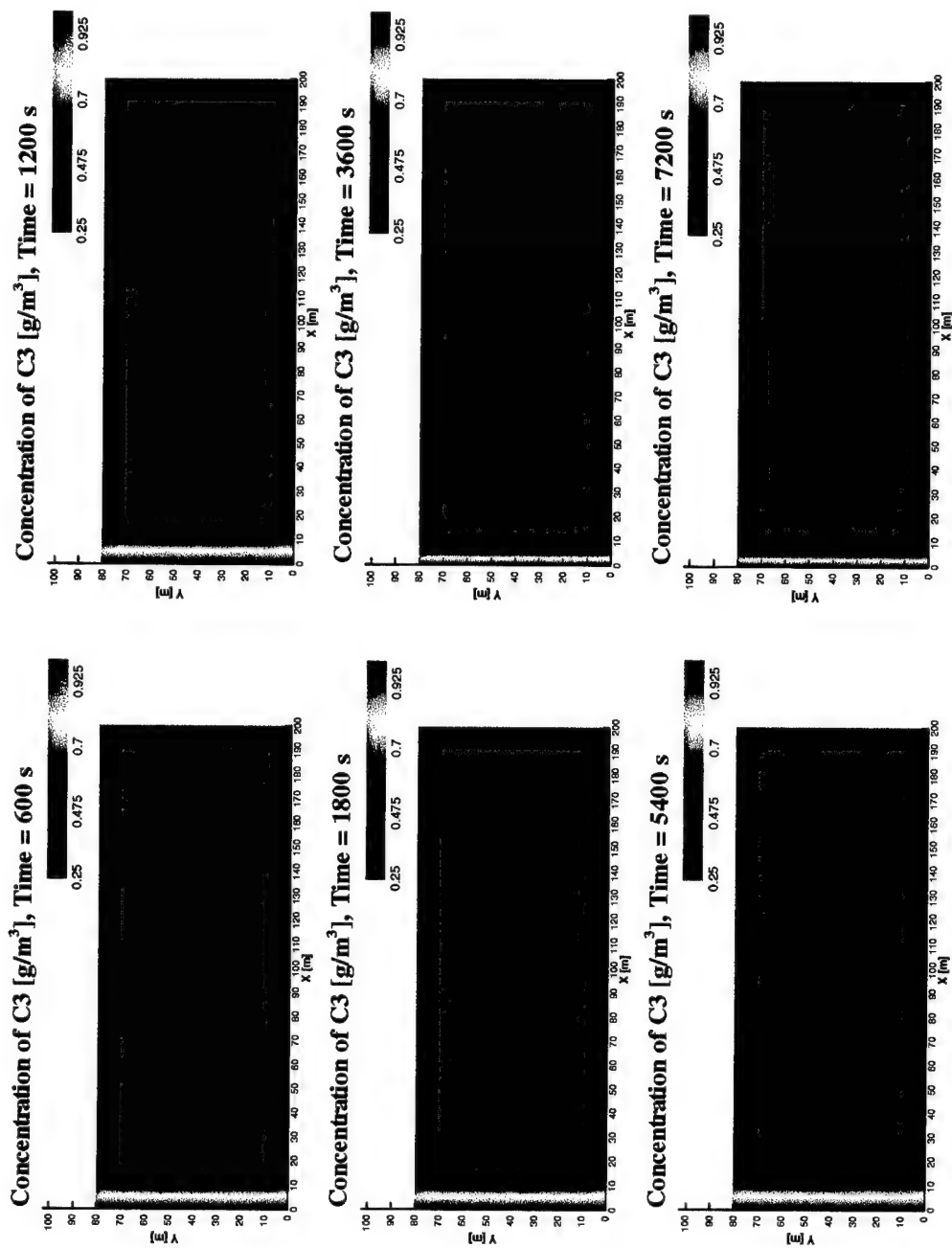


Figure 4.34. Concentration of the third dissolved chemical at various times for the example of 2-D overland flow and transport.

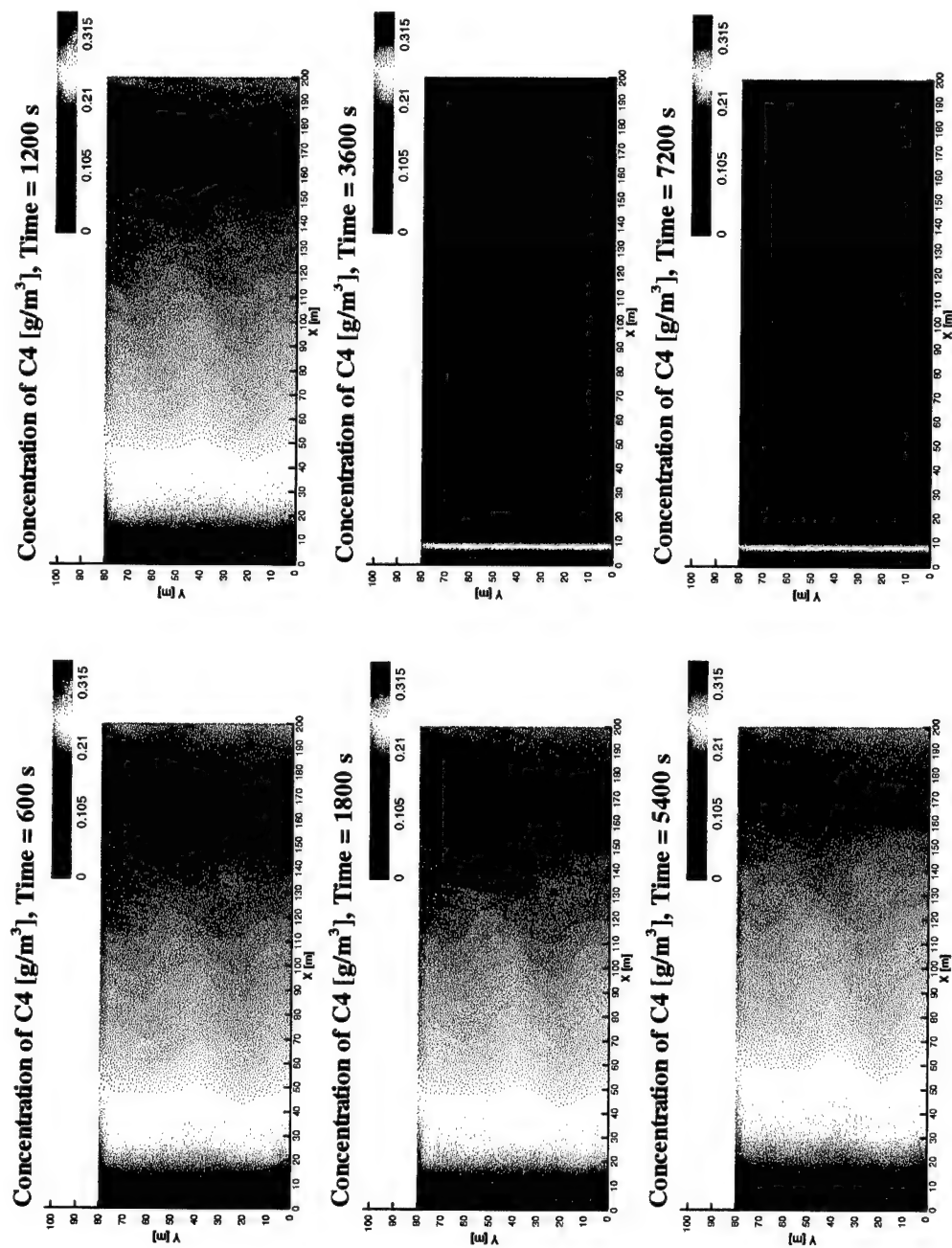


Figure 4.35. Concentration of the fourth dissolved chemical at various times for the example of 2-D overland flow and transport.

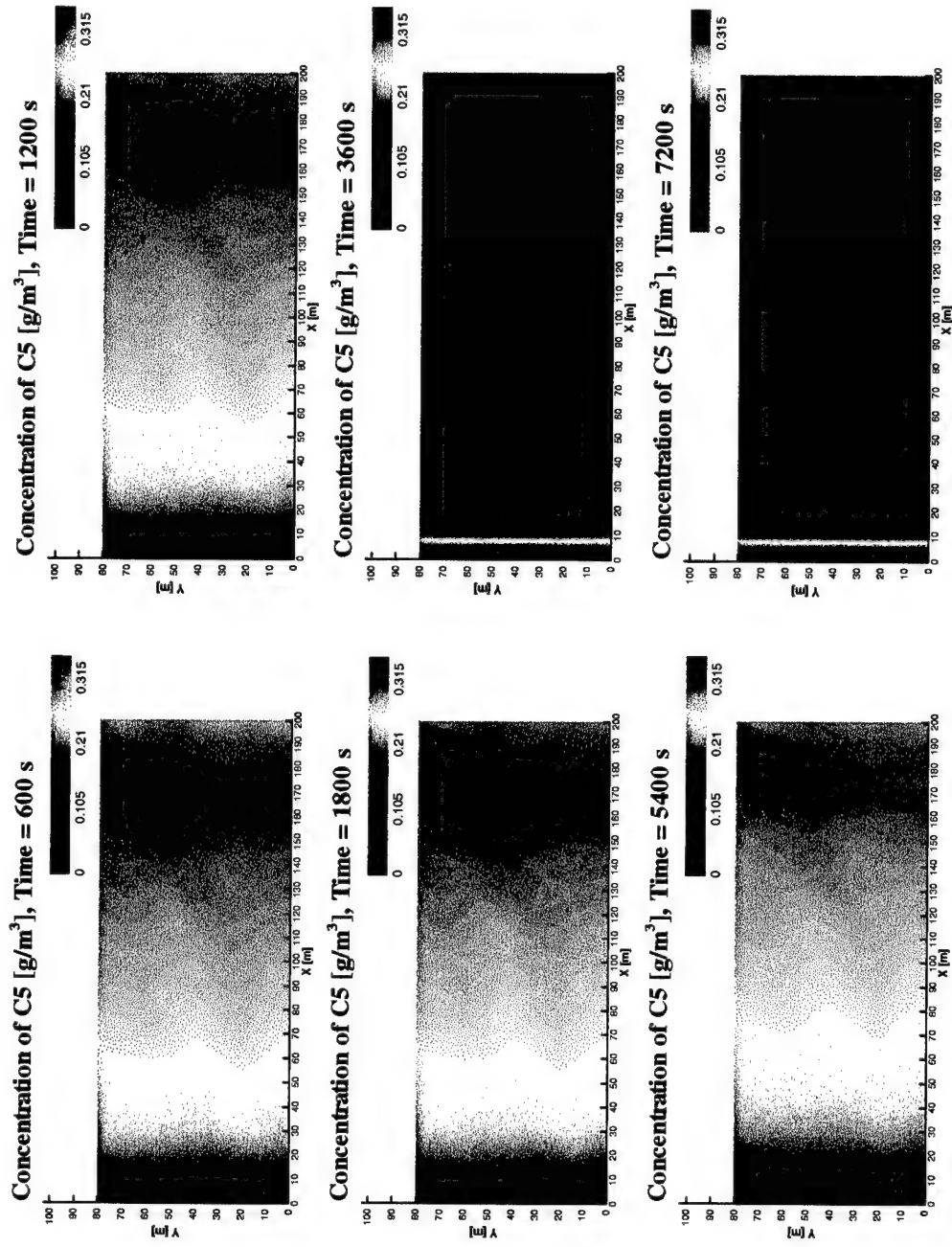


Figure 4.36. Concentration of the fifth dissolved chemical at various times for the example of 2-D overland flow and transport.

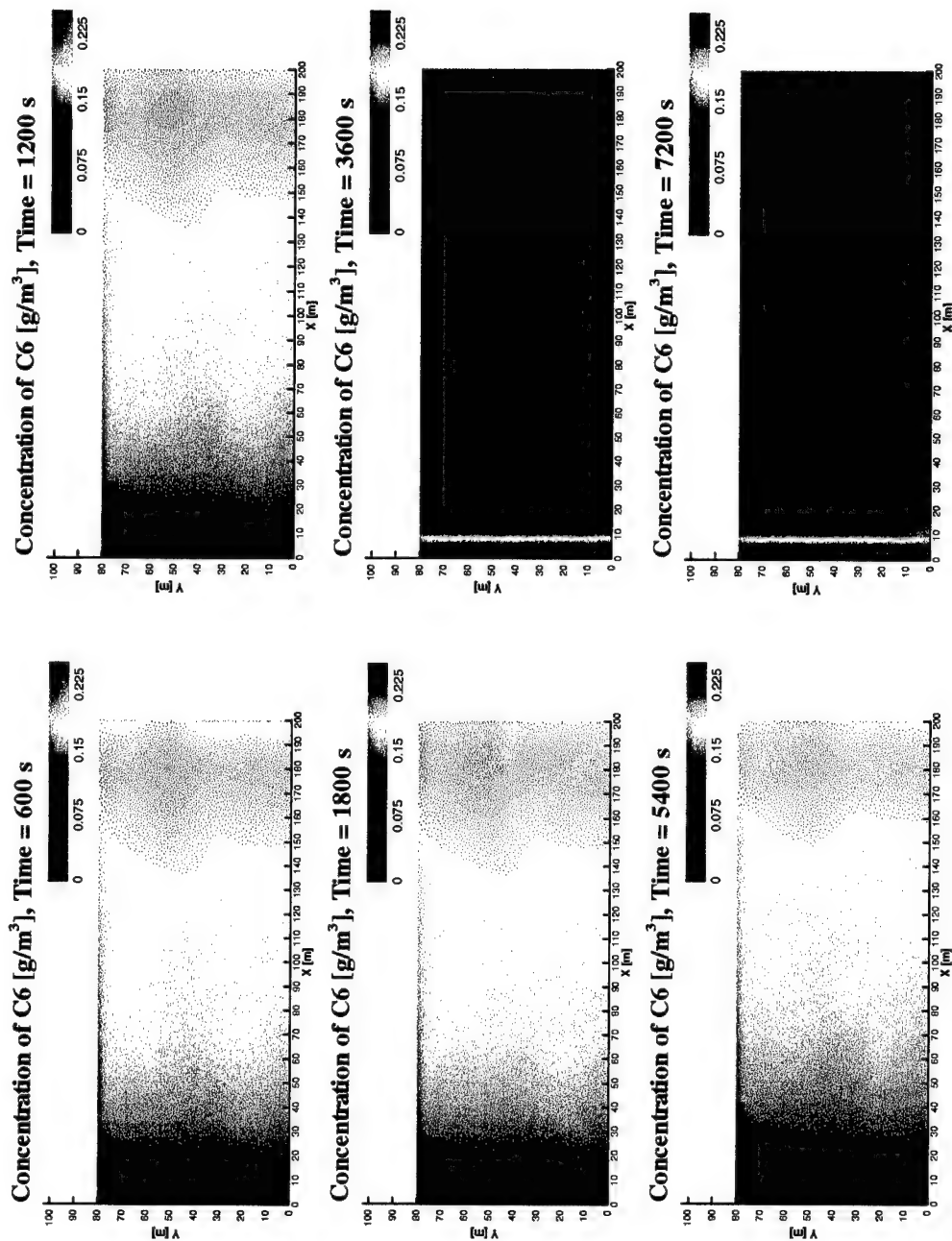


Figure 4.37. Concentration of the sixth dissolved chemical at various times for the example of 2-D overland flow and transport.

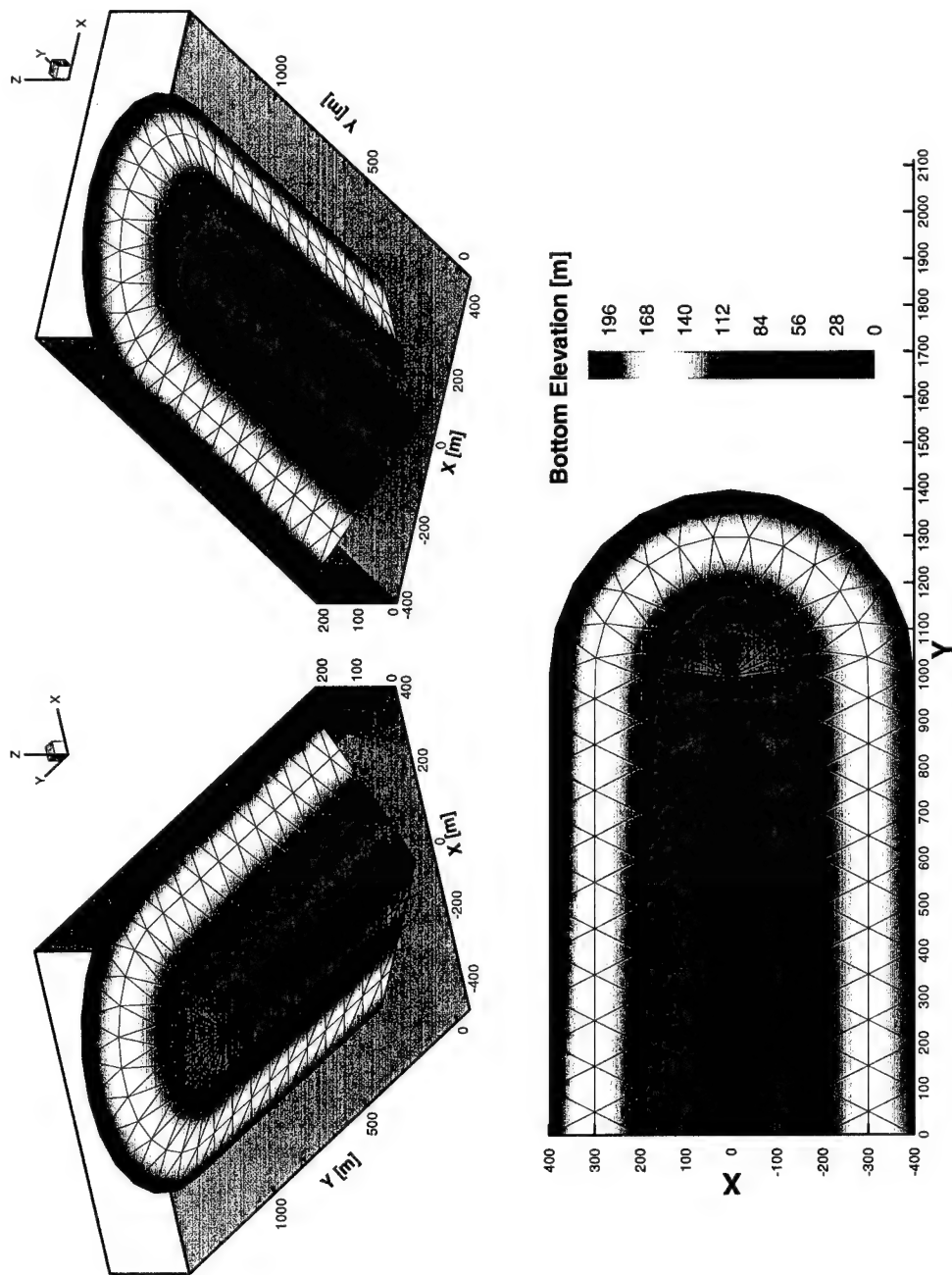


Figure 4.38. The topography and grids for the example of 1-D/2-D flow.

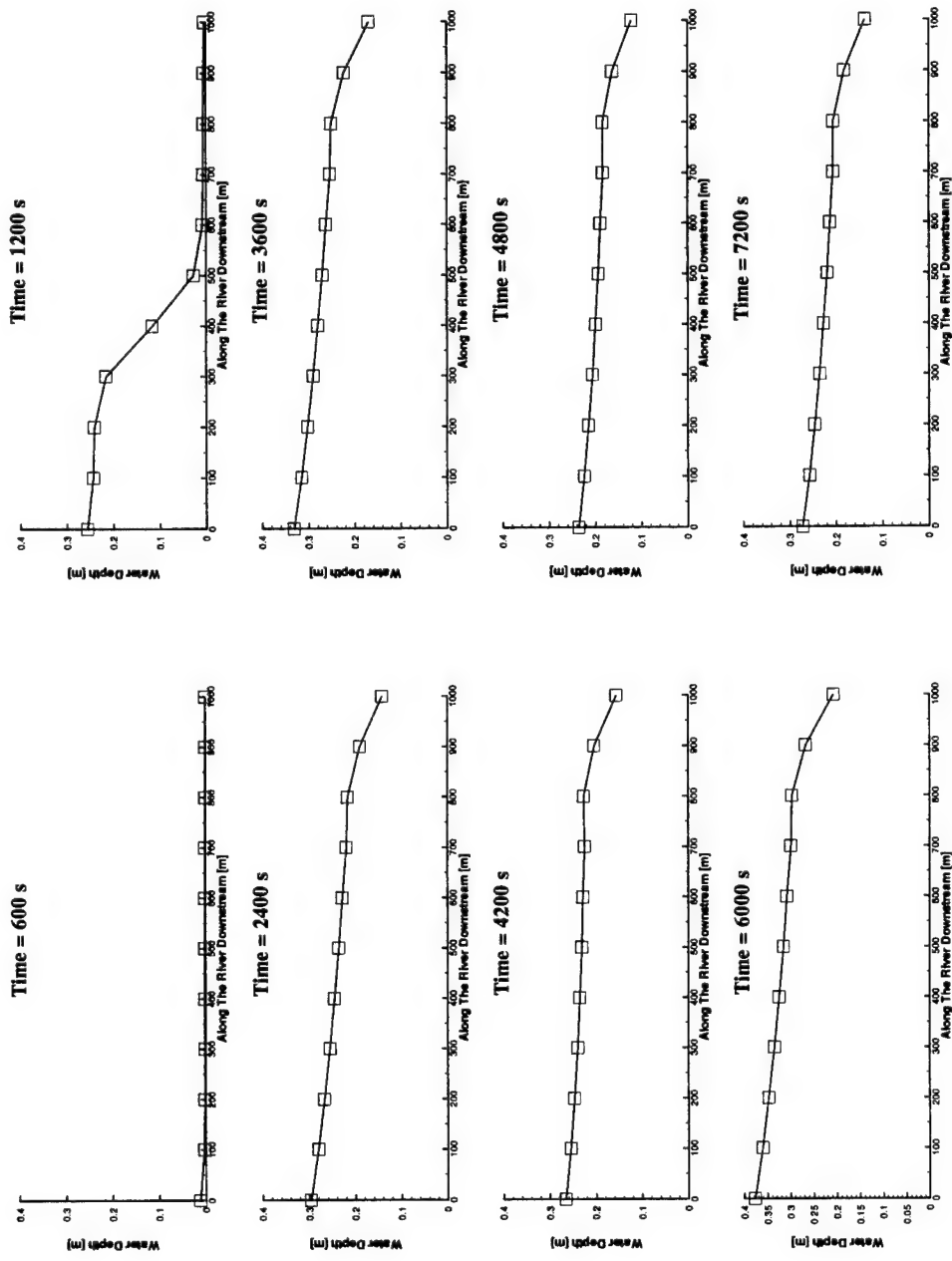


Figure 4.39. Water depth of 1-D river/stream at various times for the example of 1-D/2-D flow.

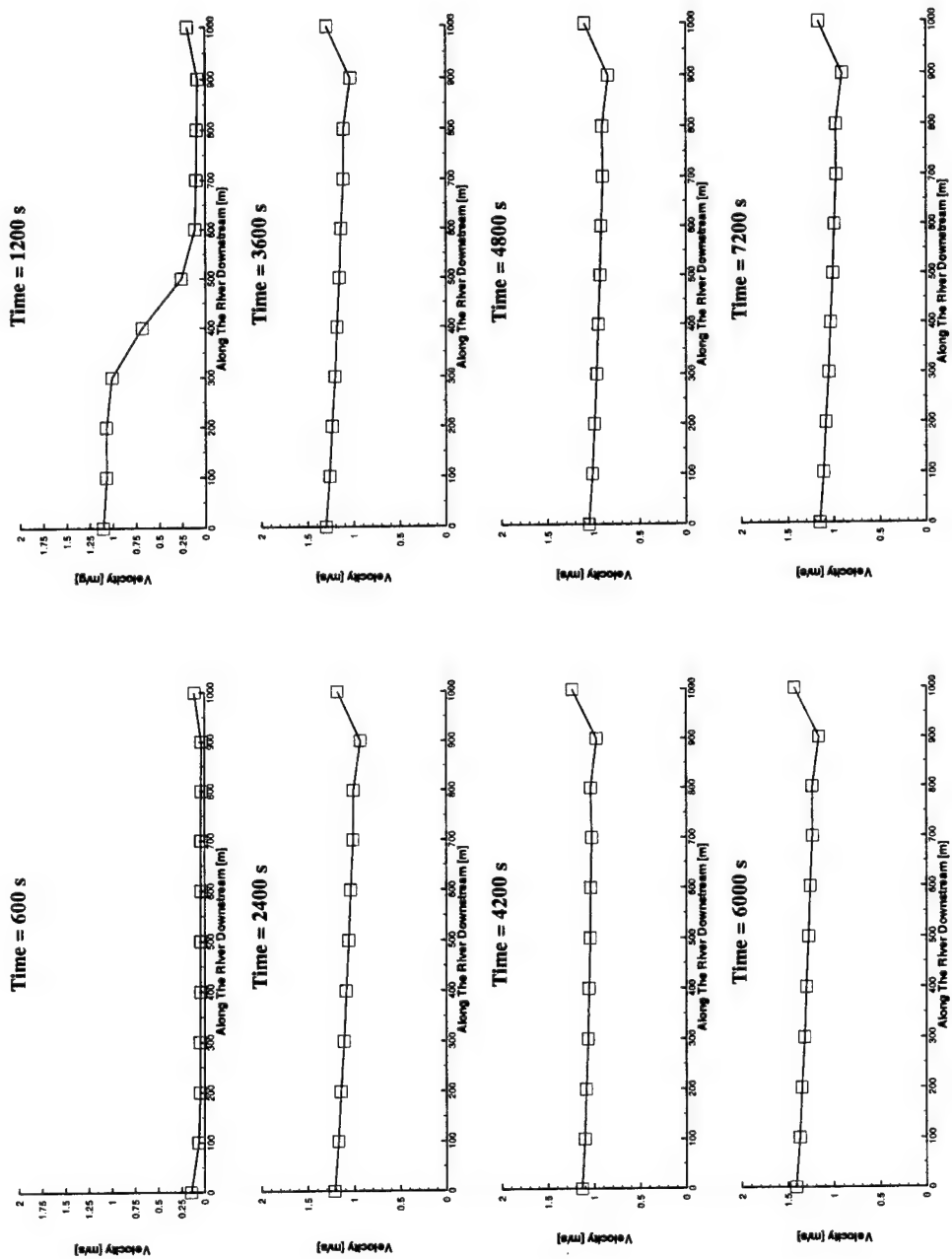


Figure 4.40. Velocity of 1-D river/stream at various times for the example of 1-D/2-D flow.

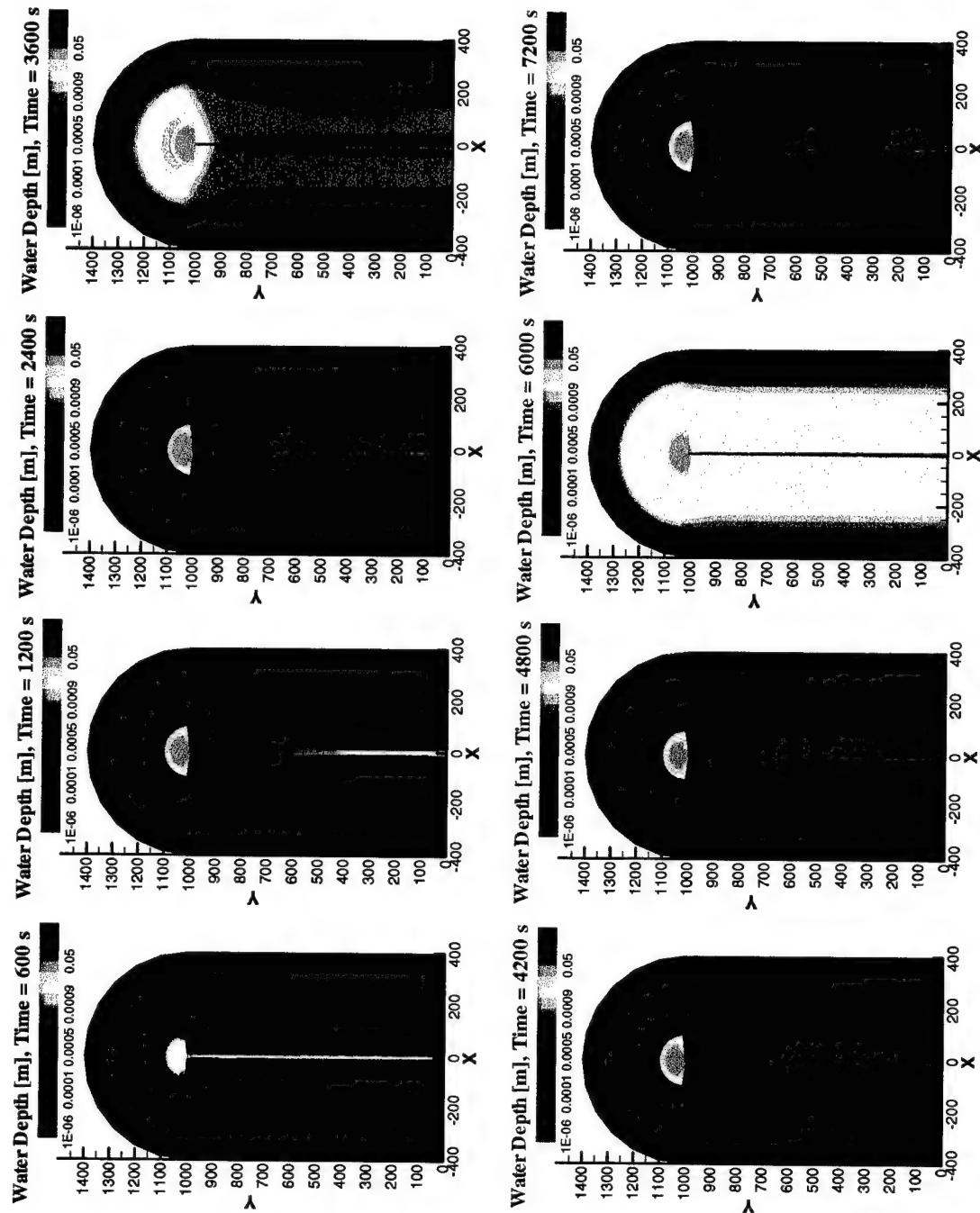


Figure 4.41. Water depth of 2-D overland at various times for the example of 1-D/2-D flow.

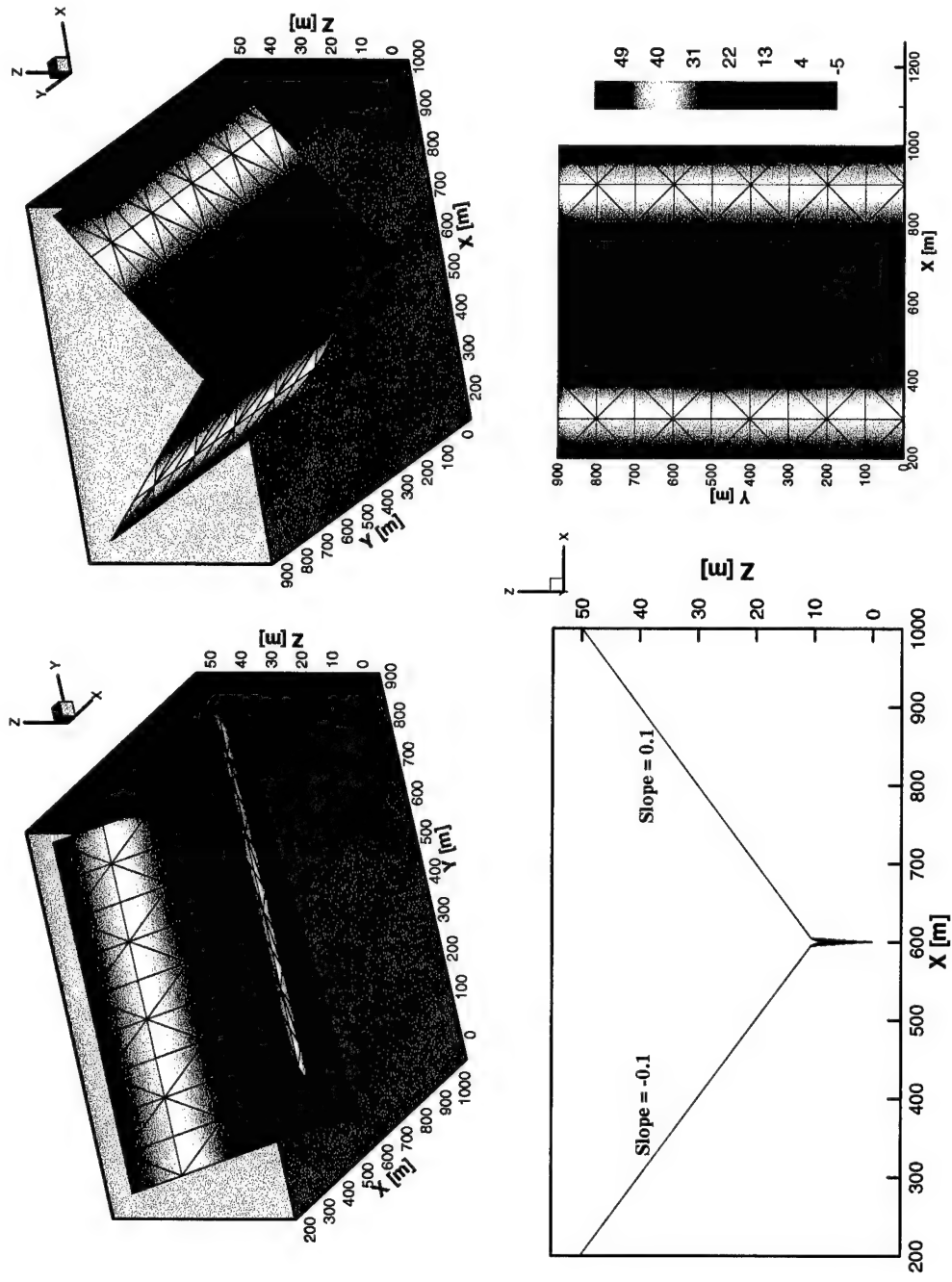


Figure 4.42. The topography and grids for the example of 1-D/2-D flow and transport.

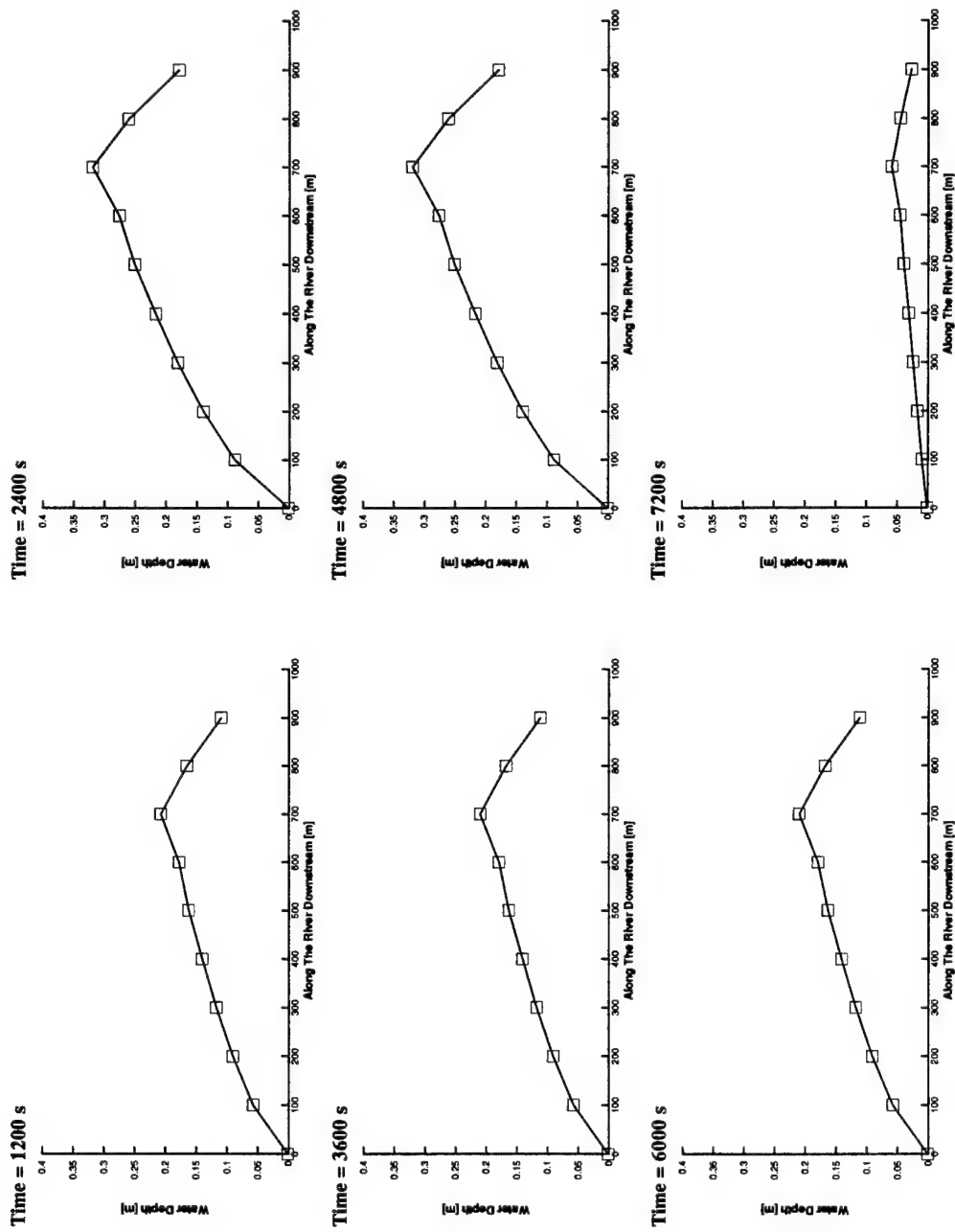


Figure 4.43. Water depth of 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

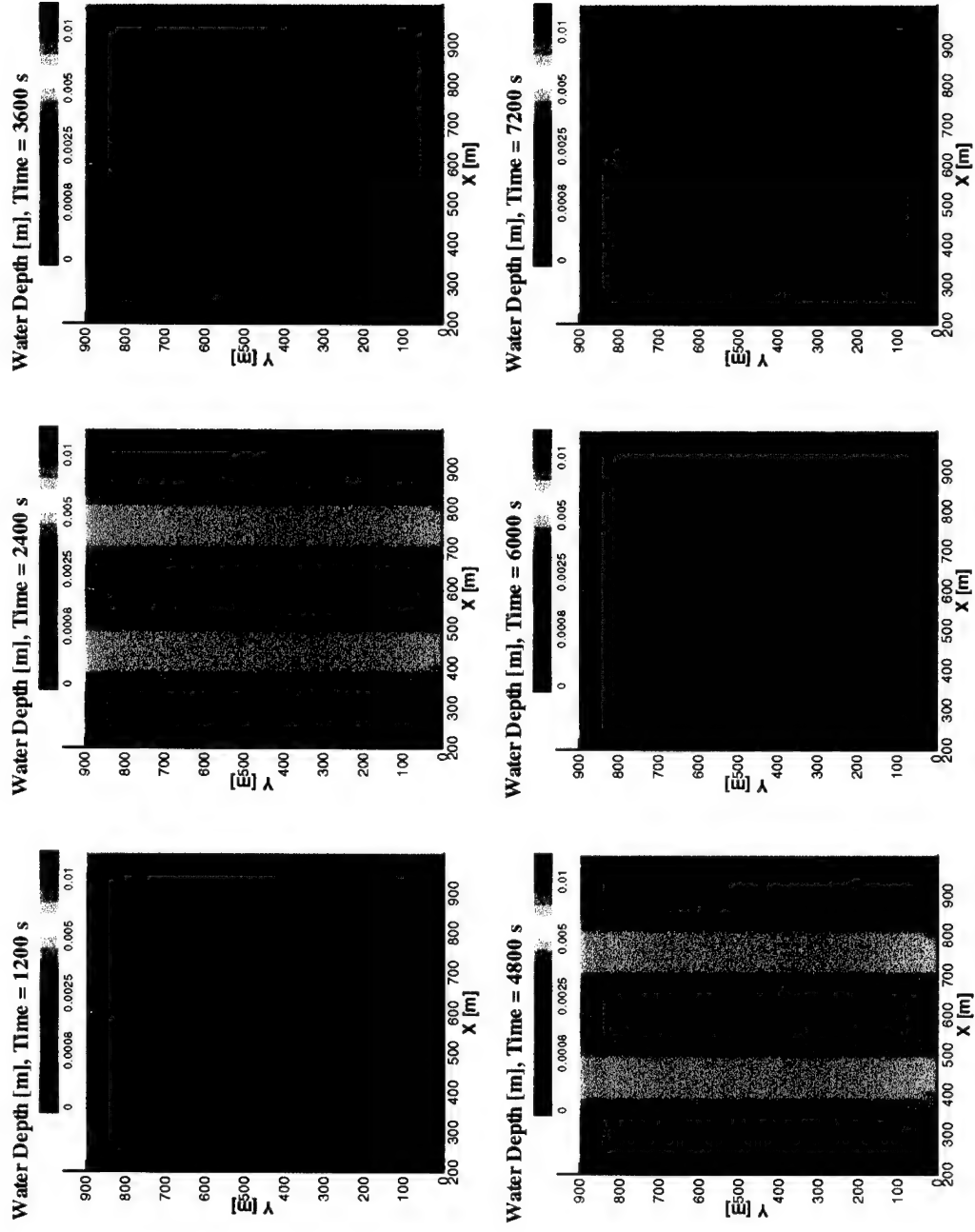


Figure 4.44. Water depth contour of 2-D overlaid at various times for the example of 1-D/2-D flow and transport.

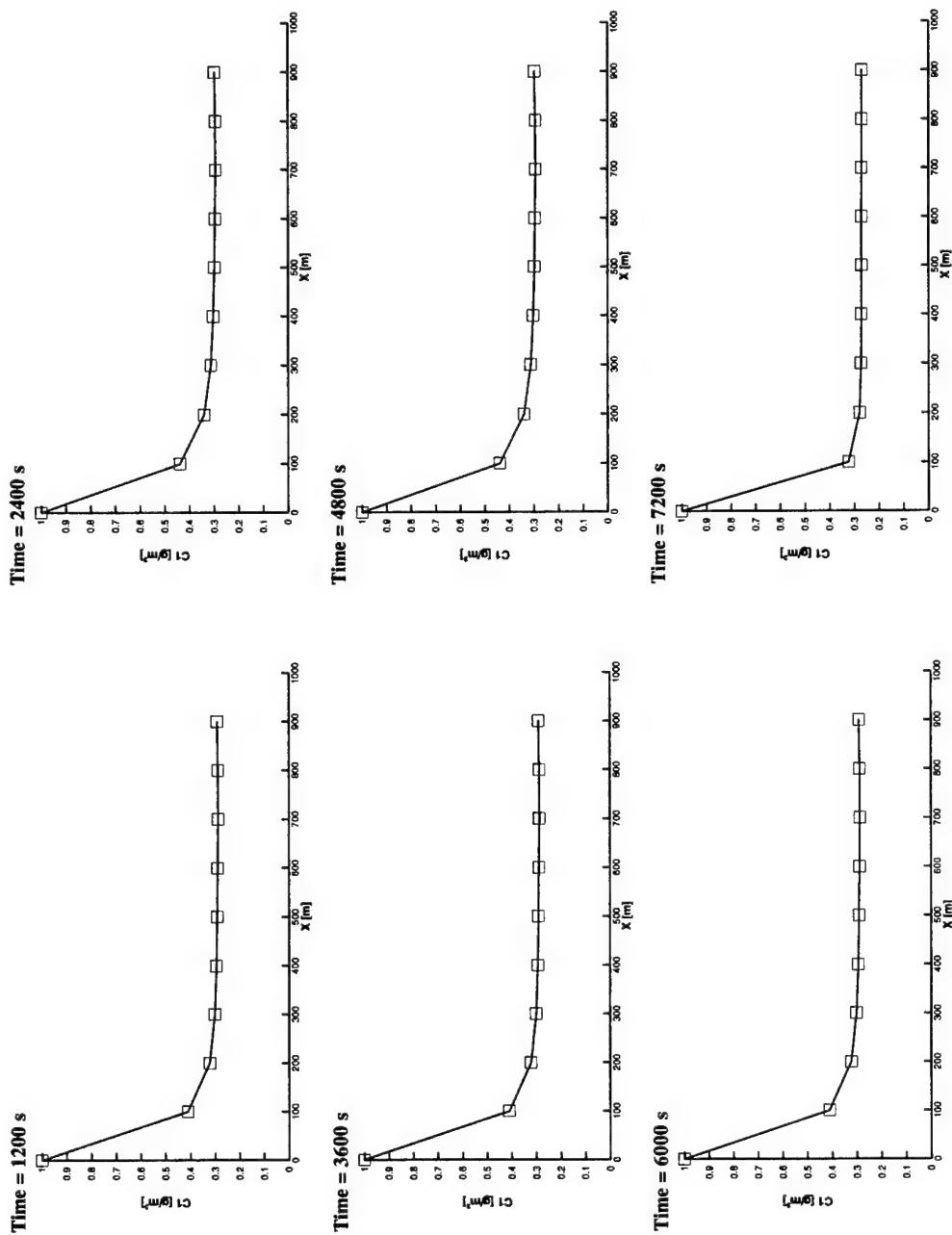


Figure 4.45. Concentration of the first dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

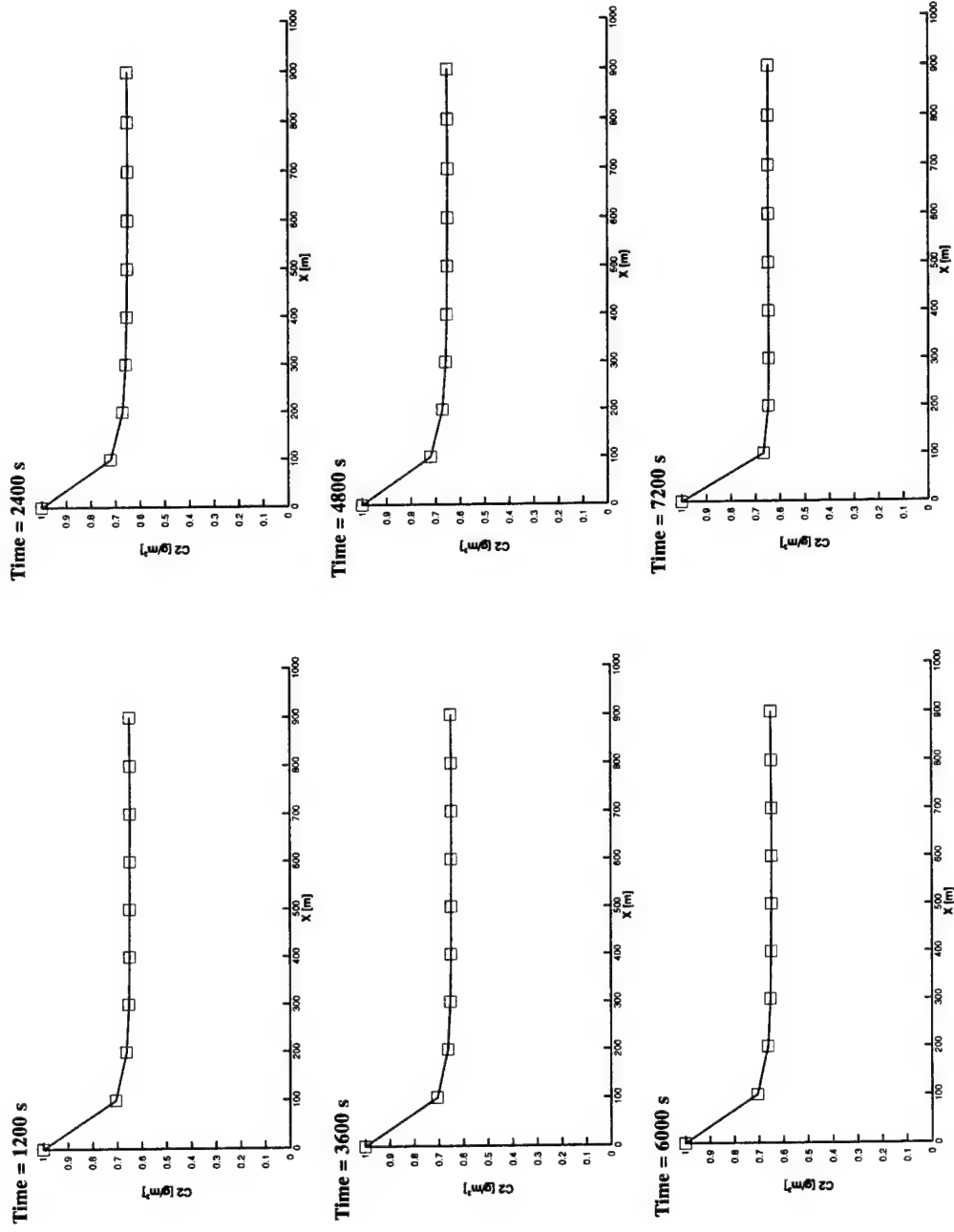


Figure 4.46. Concentration of the second dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

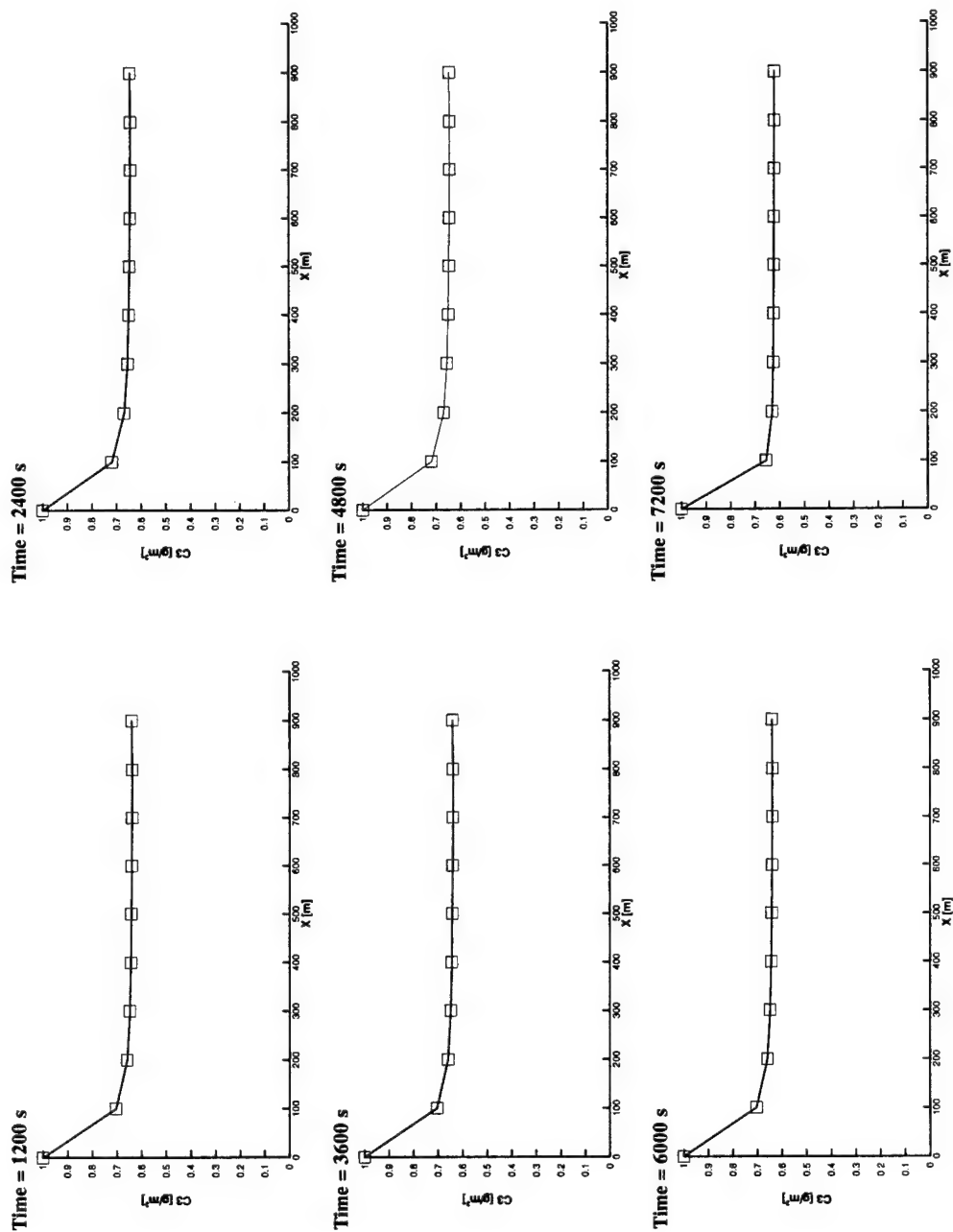


Figure 4.47. Concentration of the third dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

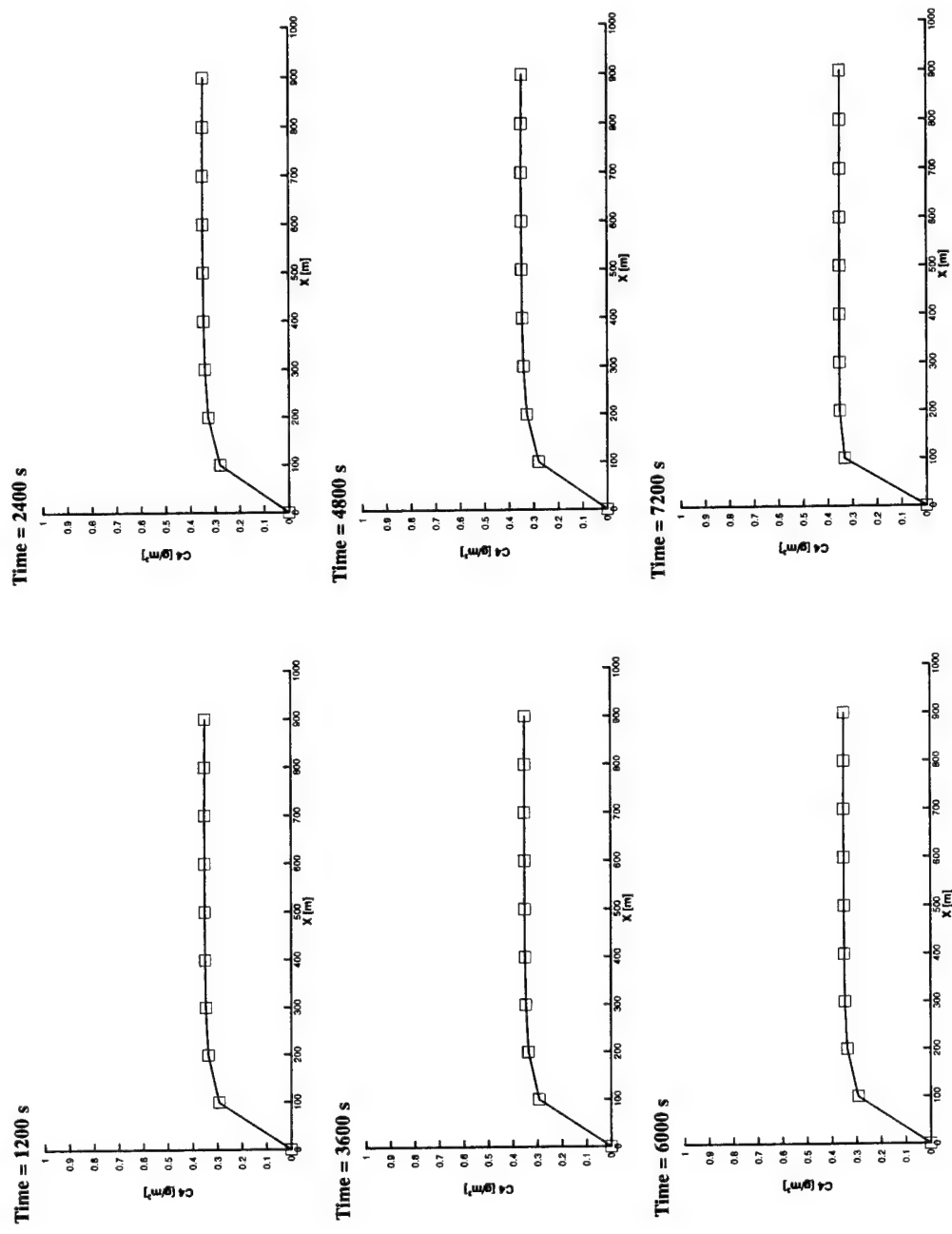


Figure 4.48. Concentration of the fourth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

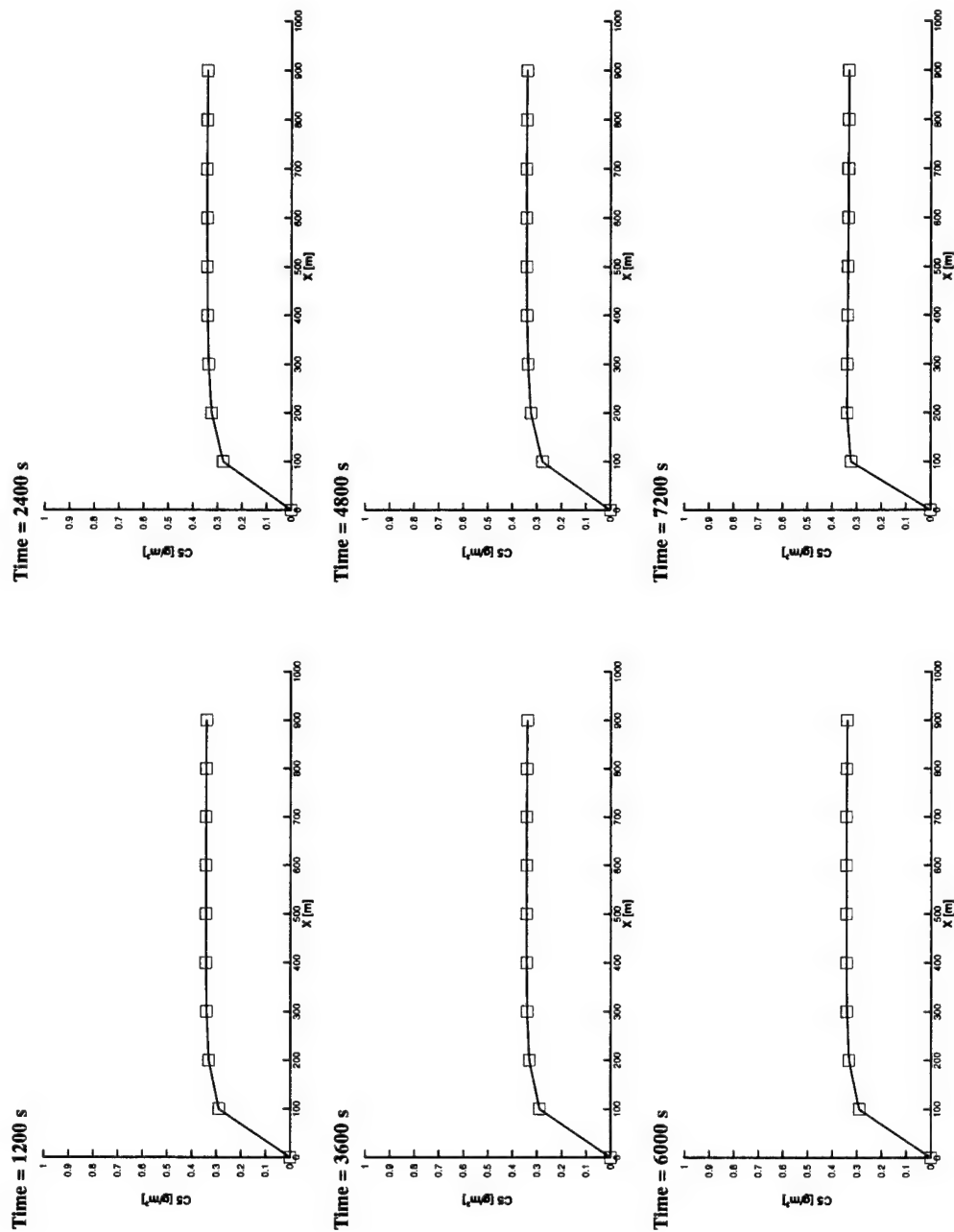


Figure 4.49. Concentration of the fifth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

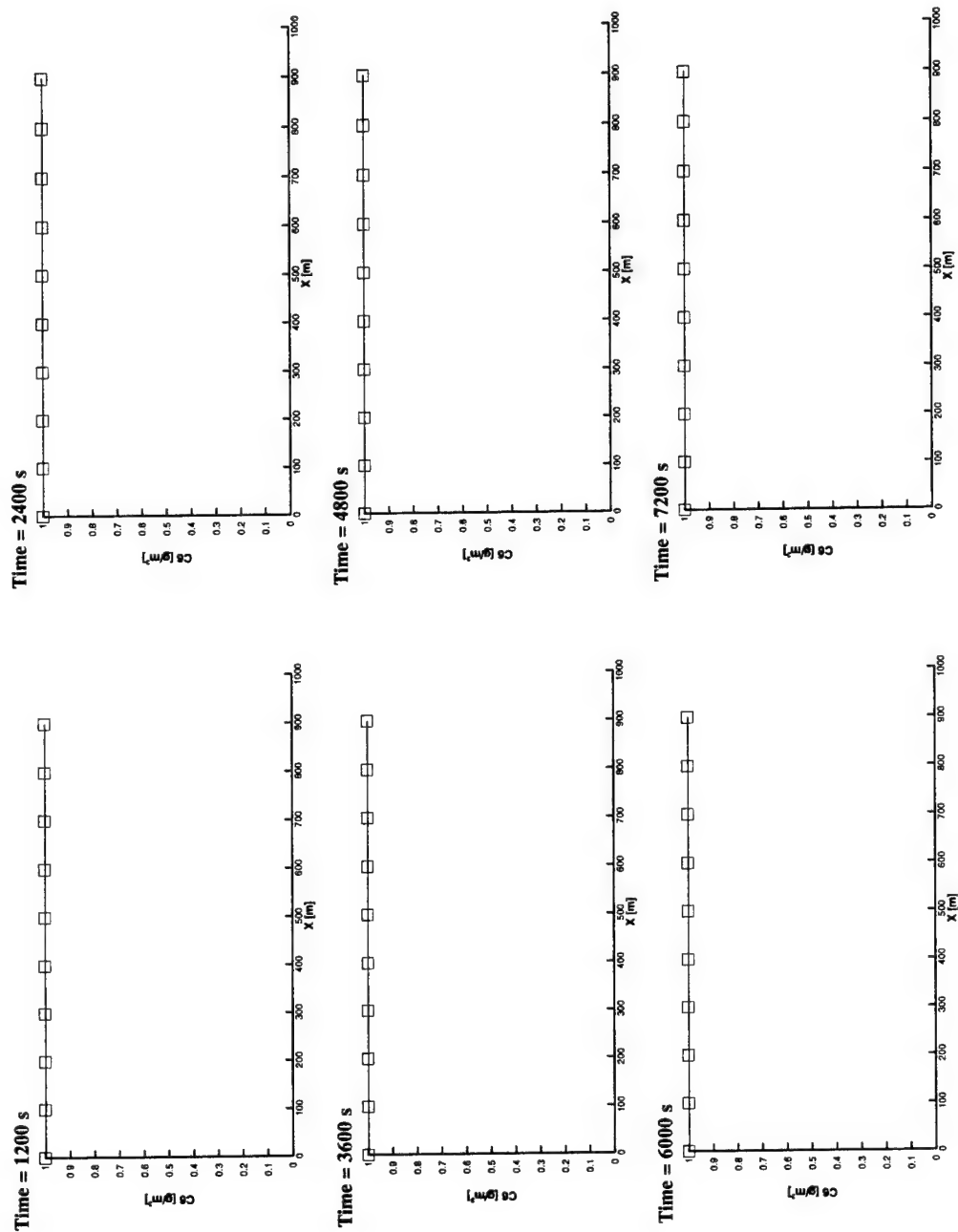


Figure 4.50. Concentration of the sixth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

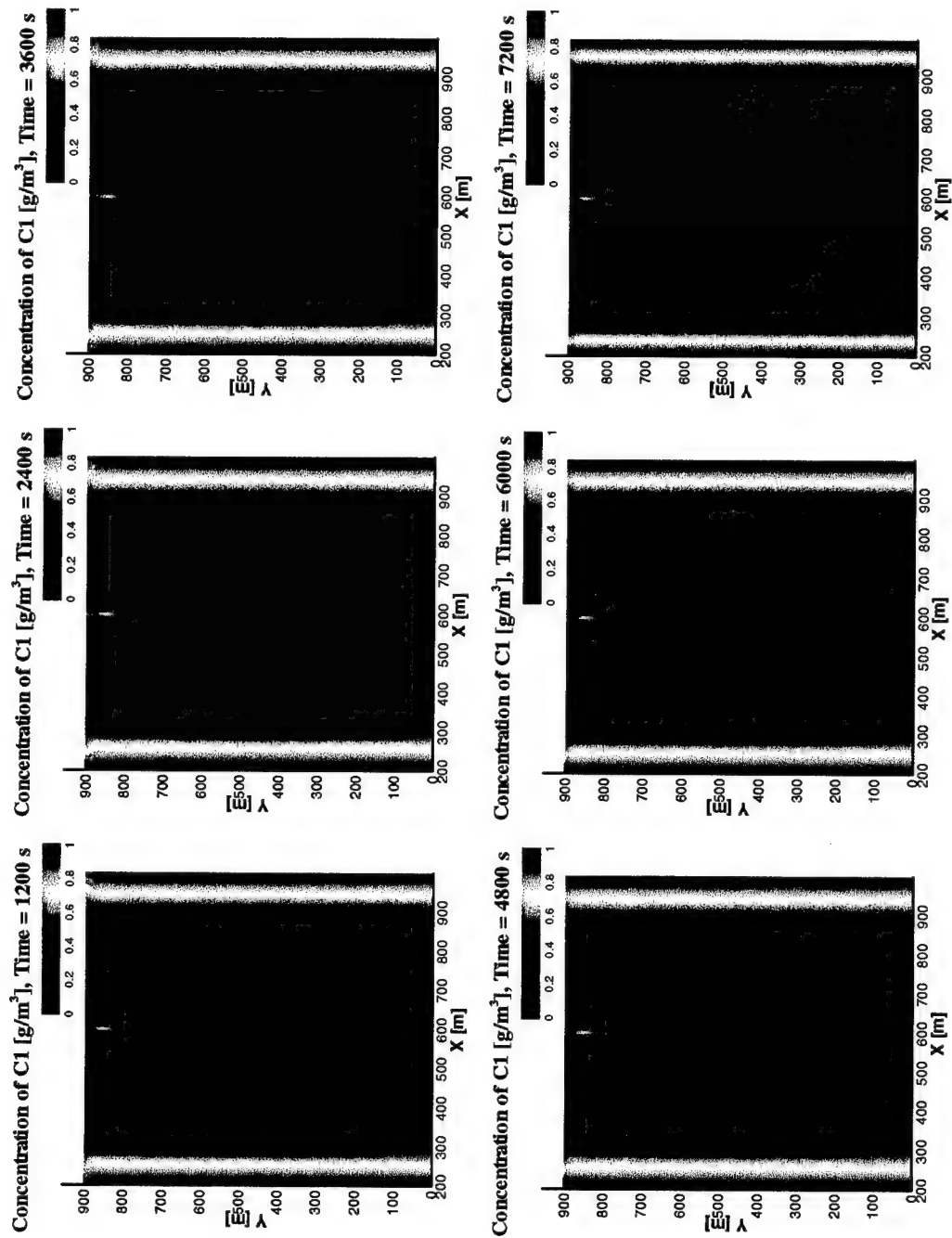


Figure 4.51. Concentration of the first dissolved chemical in 2-D overlaid at various times for the example of 1-D/2-D flow and transport.

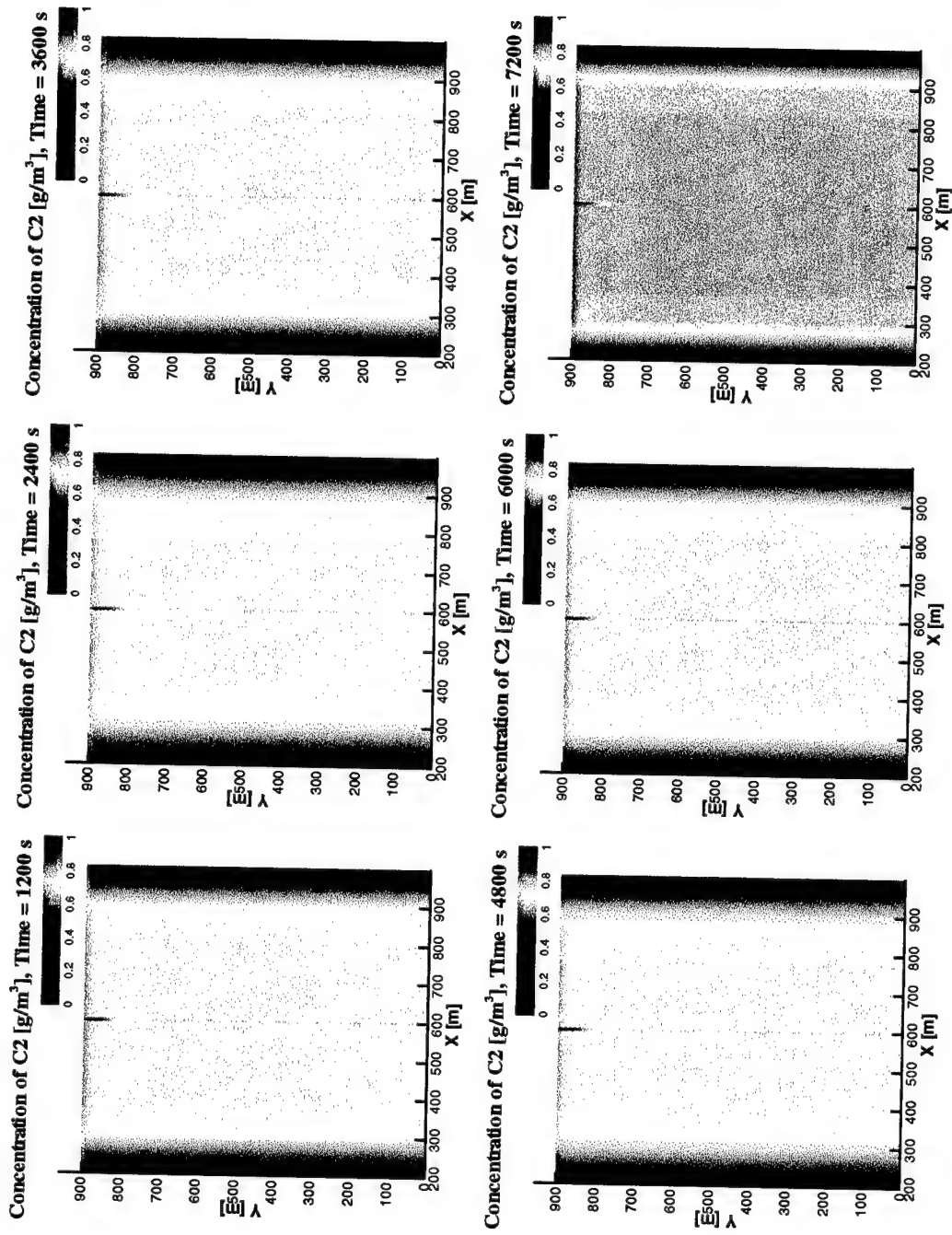


Figure 4.52. Concentration of the second dissolved chemical in 2-D overlaid at various times for the example of 1-D/2-D flow and transport.

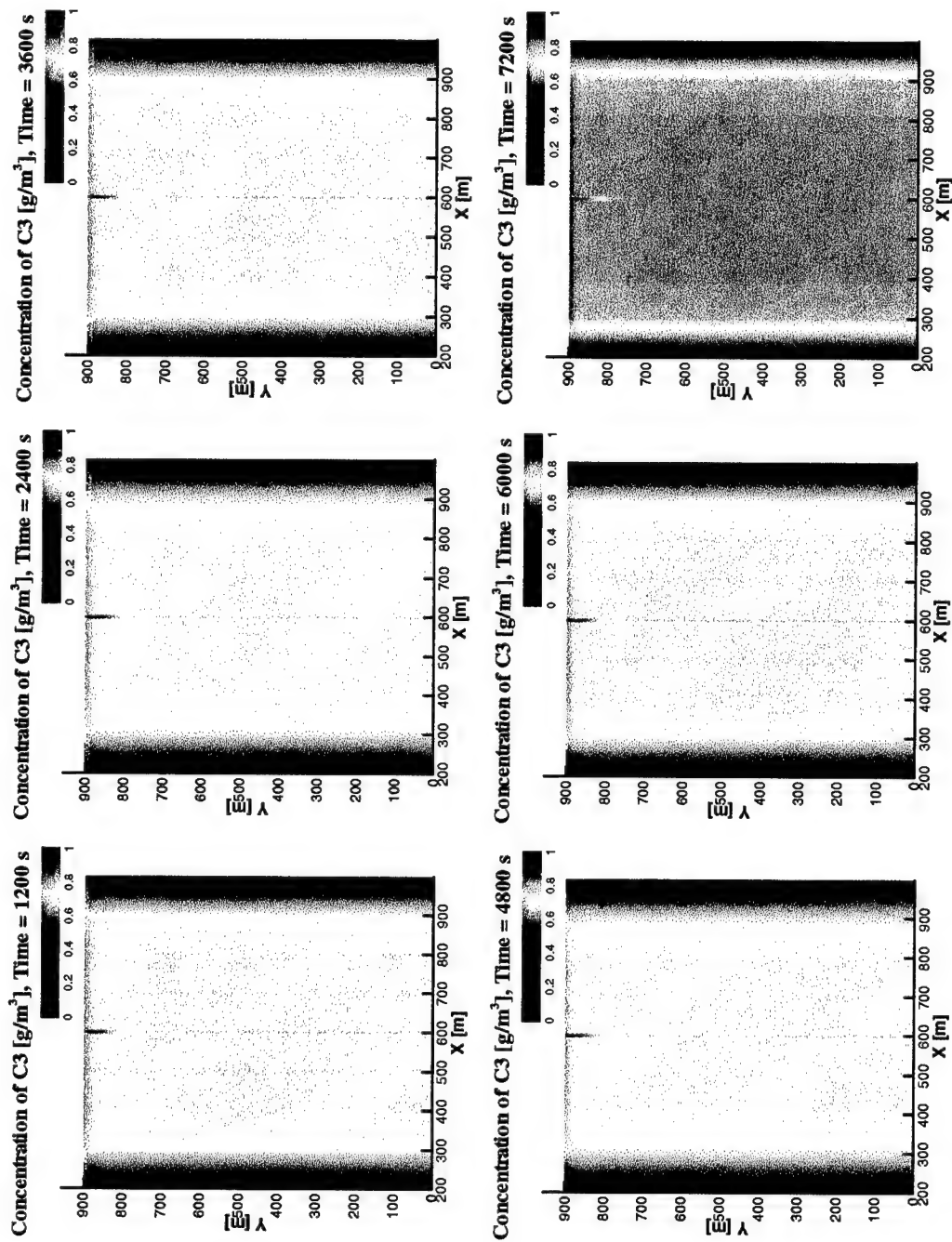


Figure 4.53. Concentration of the third dissolved chemical in 2-D overlaid at various times for the example of 1-D/2-D flow and transport.

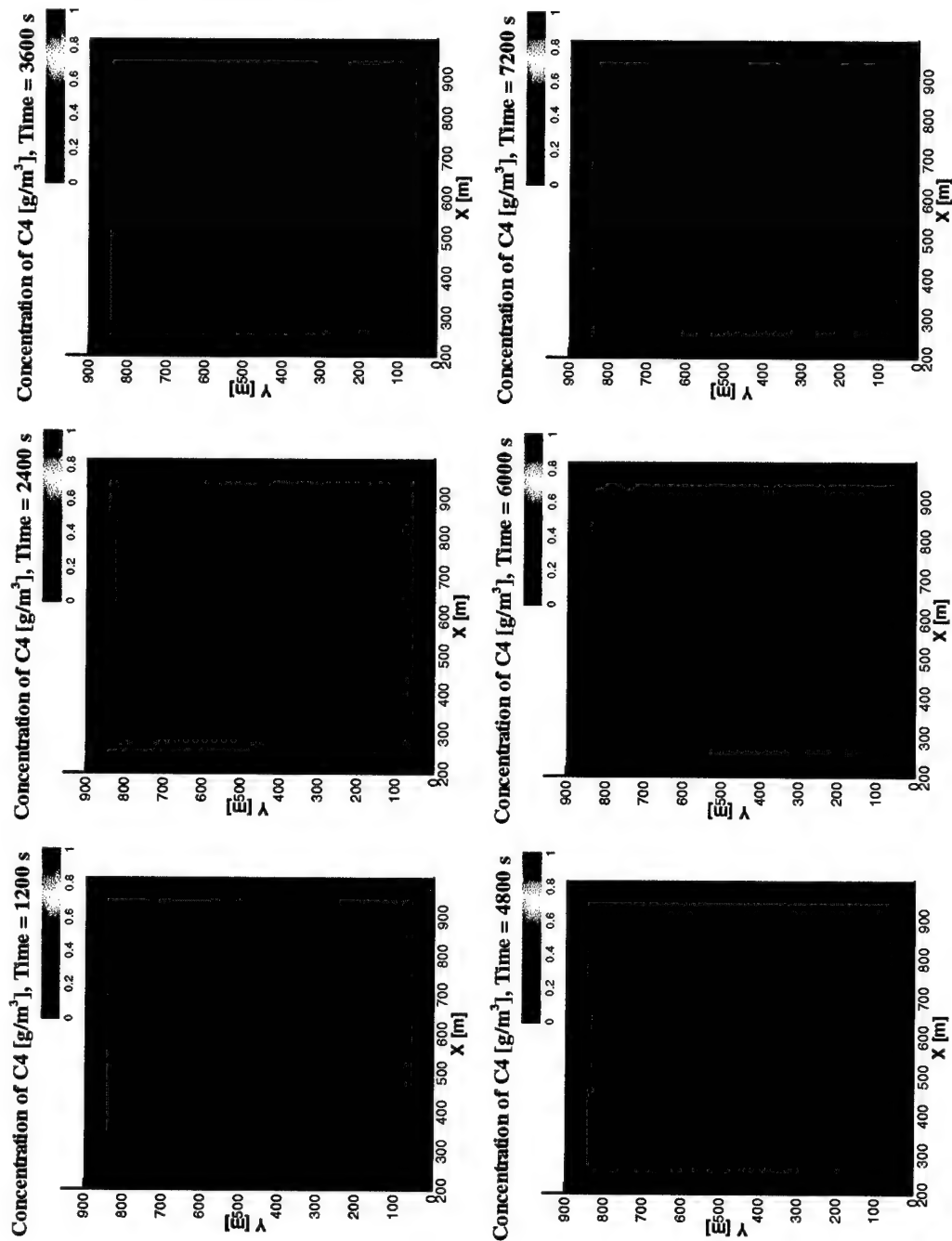


Figure 4.54. Concentration of the fourth dissolved chemical in 2-D overlaid at various times for the example of 1-D/2-D flow and transport.

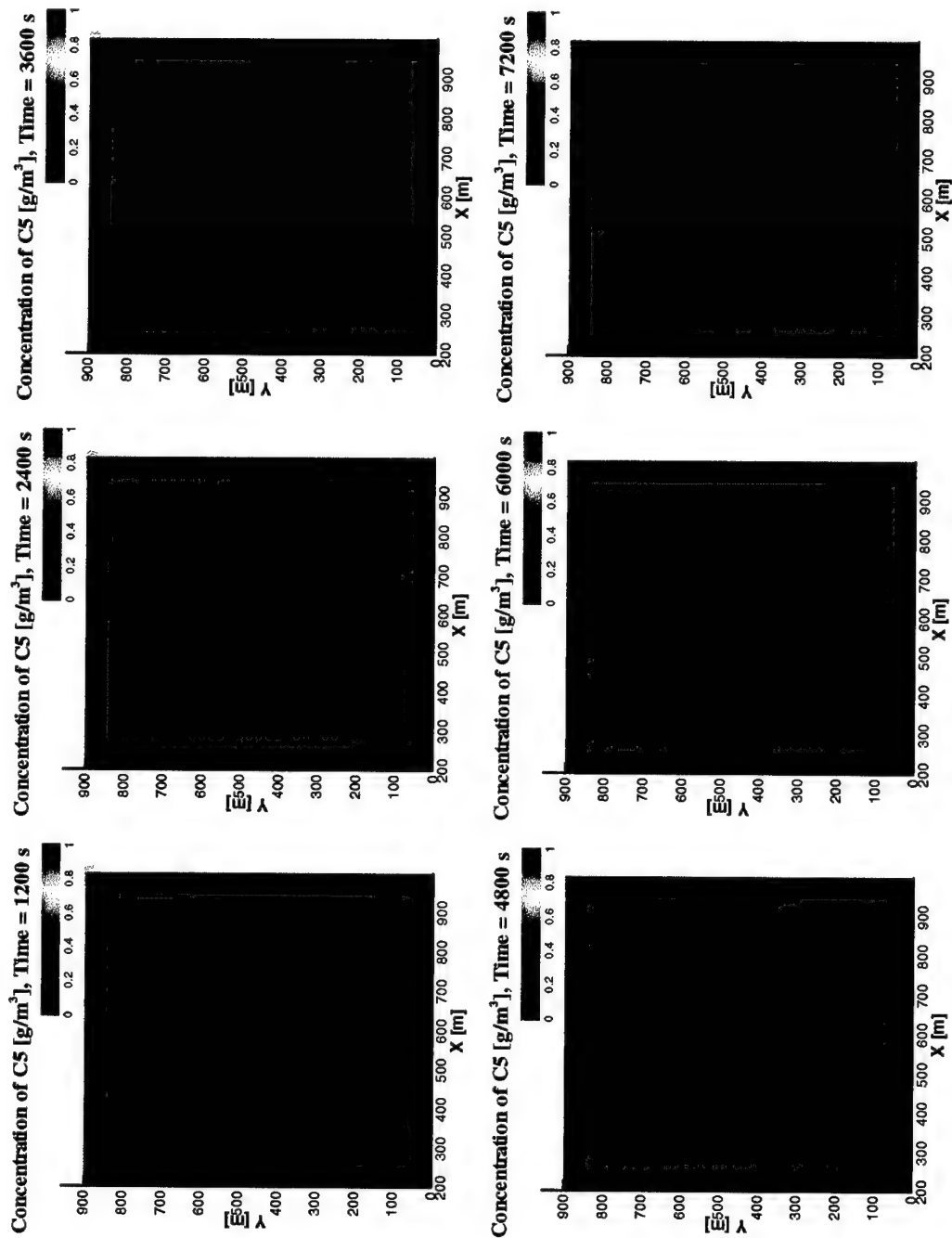


Figure 4.55. Concentration of the fifth dissolved chemical in 2-D overlaid at various times for the example of 1-D/2-D flow and transport.

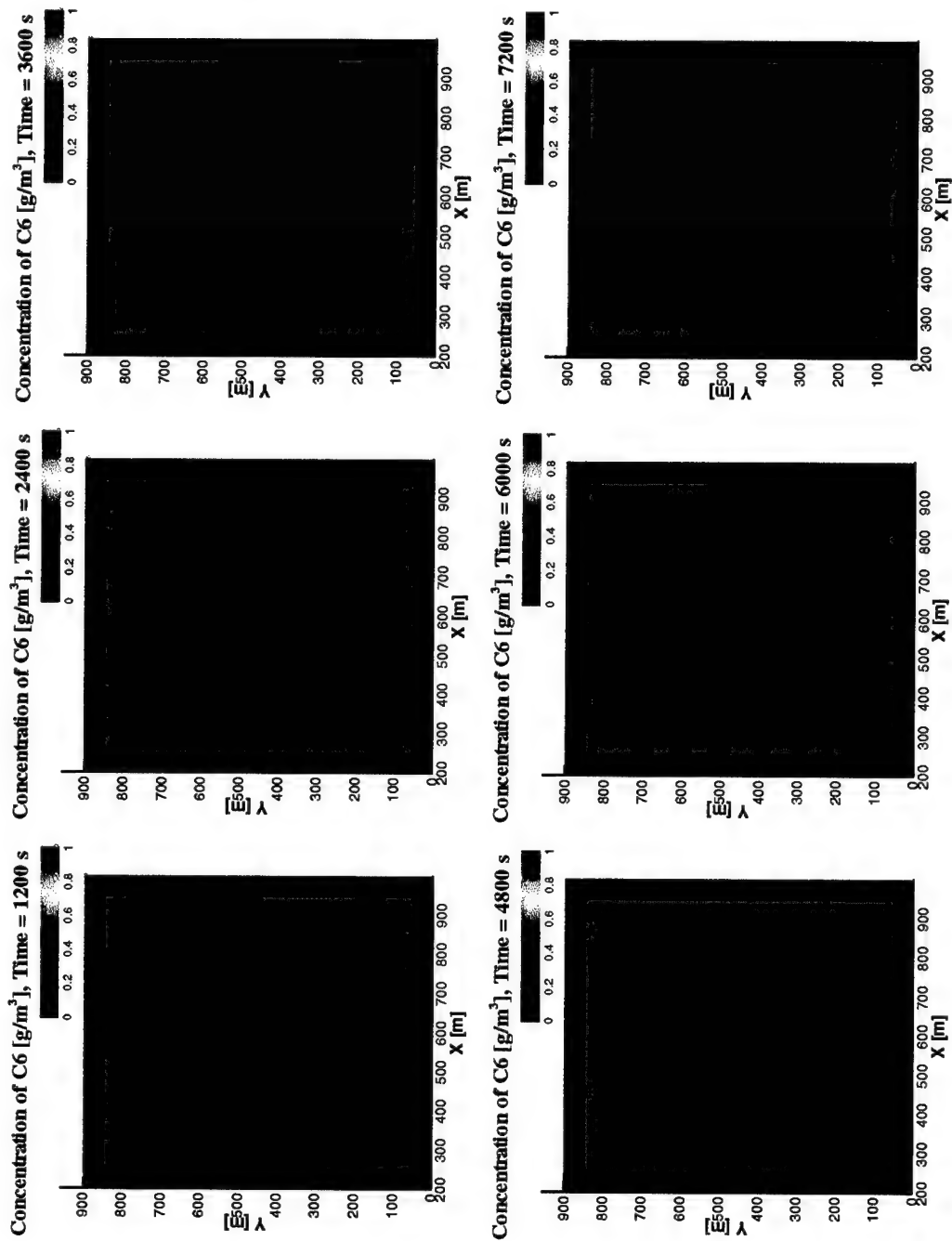


Figure 4.56. Concentration of the sixth dissolved chemical in 2-D overlaid at various times for the example of 1-D/2-D flow and transport.

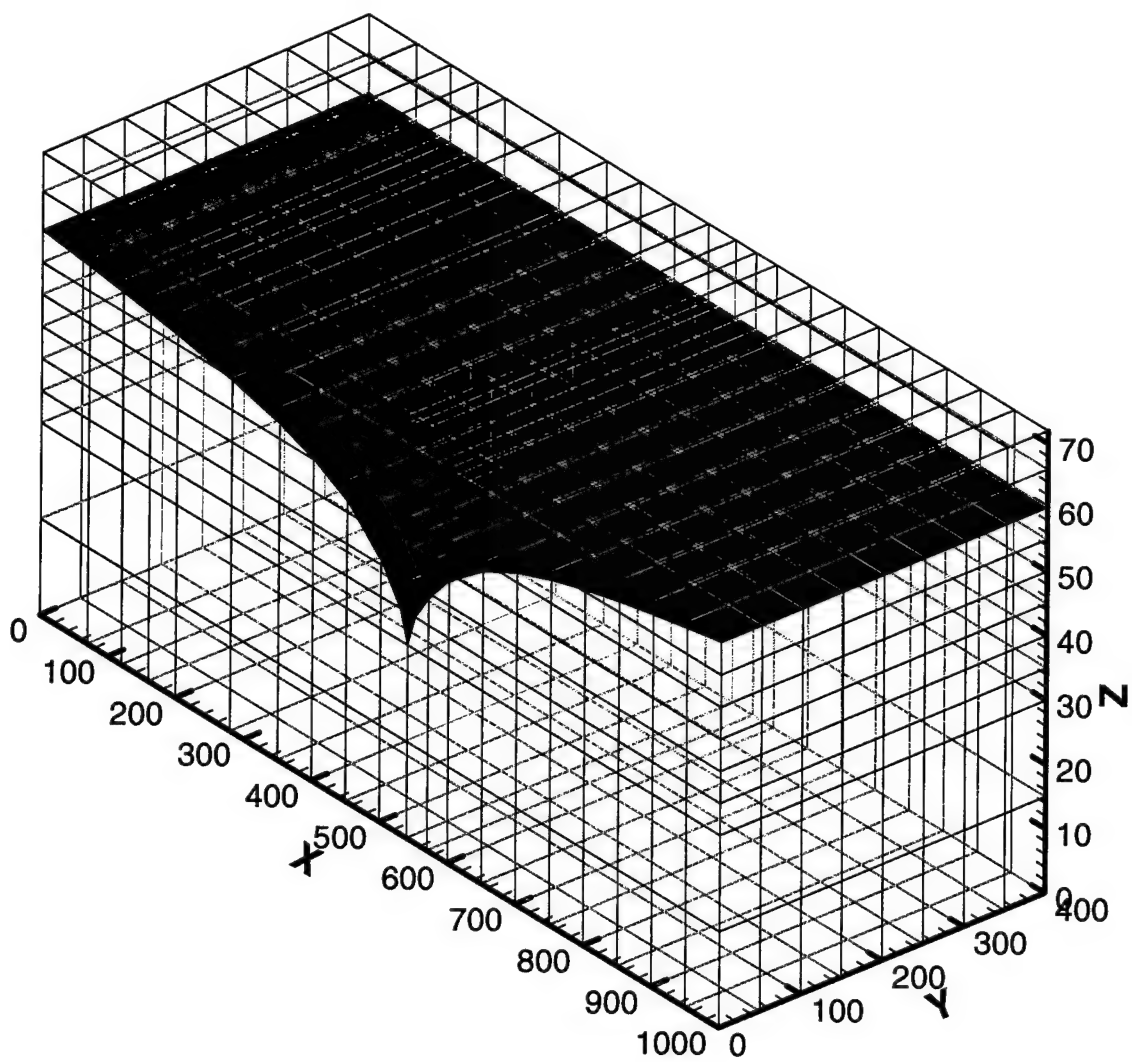


Figure 4.57. The steady-state solution of the 3-D subsurface flow example.

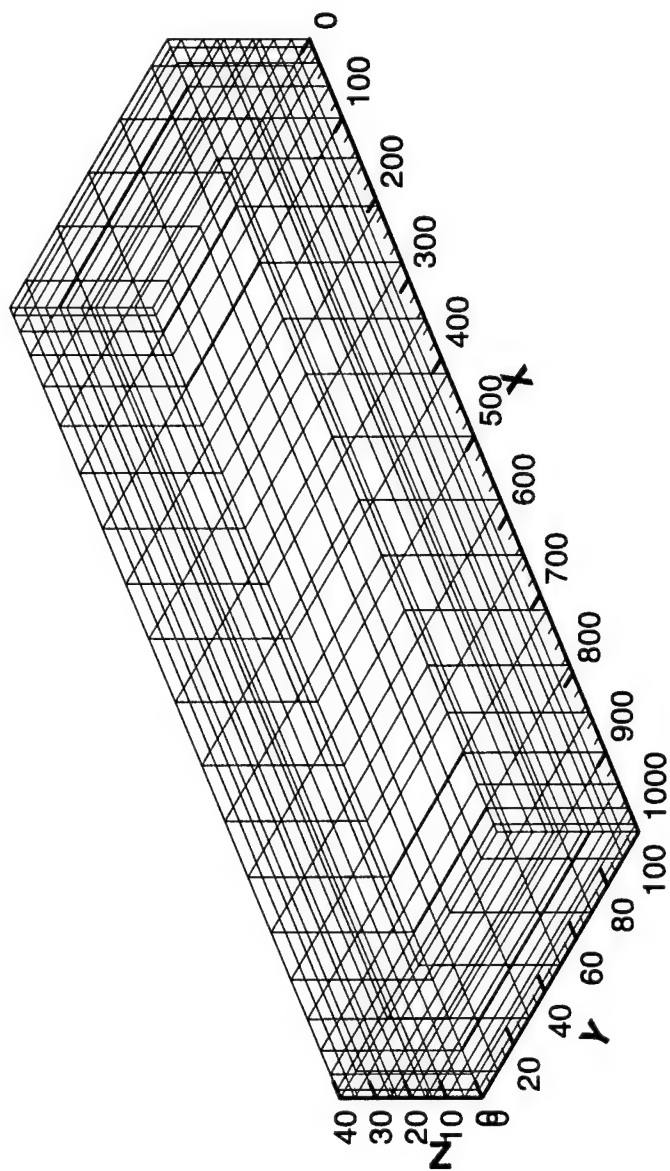


Figure 4.58. The discretization of the 3-D subsurface transport example.

Time = 60 hours

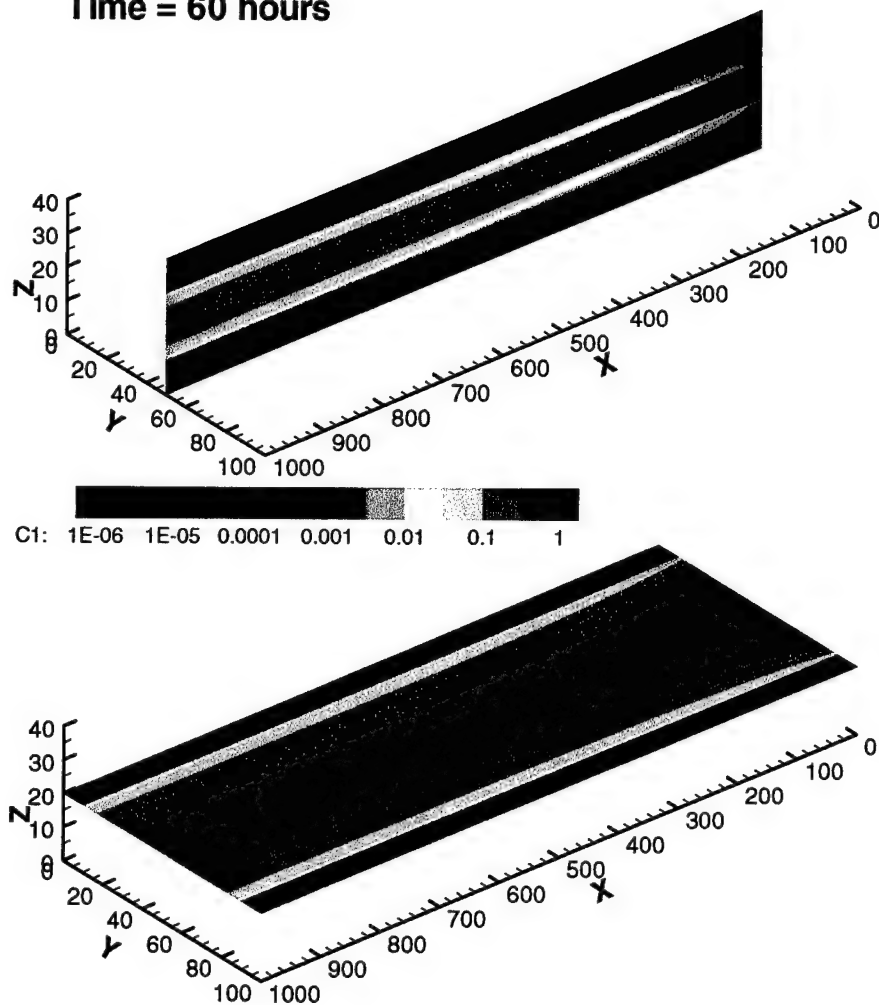


Figure 4.59. The concentration distribution of the 1st dissolved chemical [g/m³] at time = 60 hour in the 3-D transport example.

Time = 60 hours

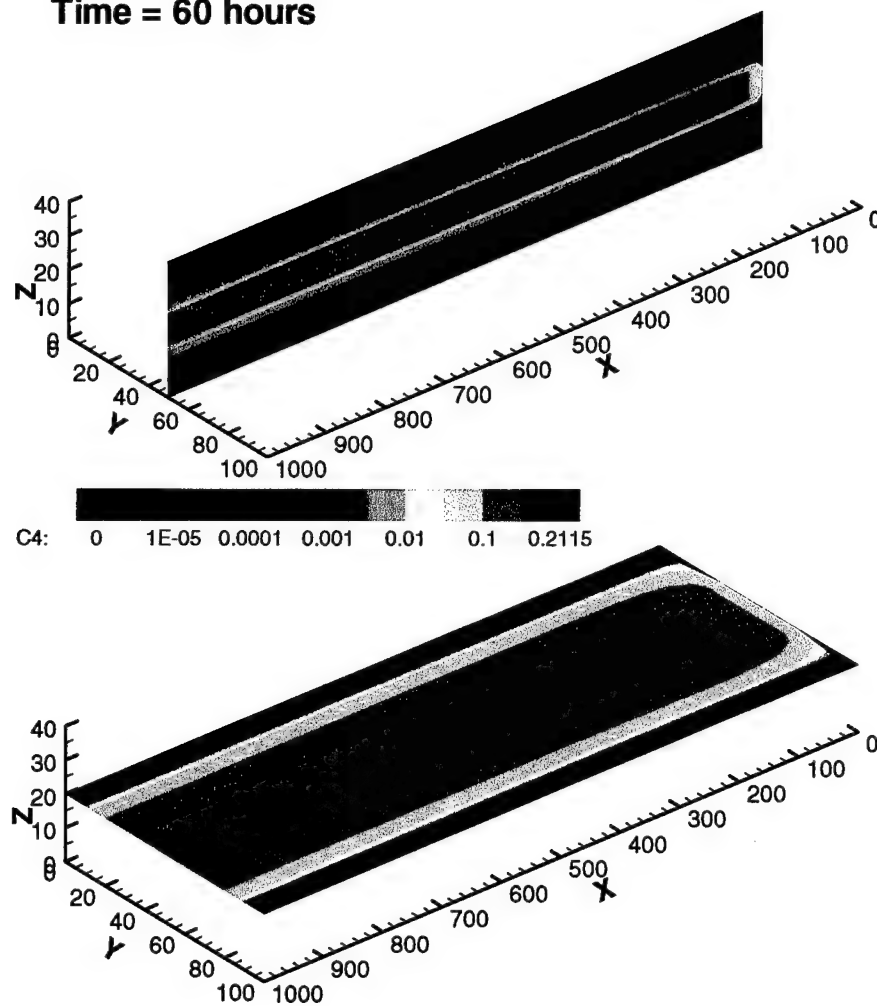


Figure 4.60. The concentration distribution of the 4th dissolved chemical [g/m³] at time = 60 hour in the 3-D transport example.

Time = 60 hours

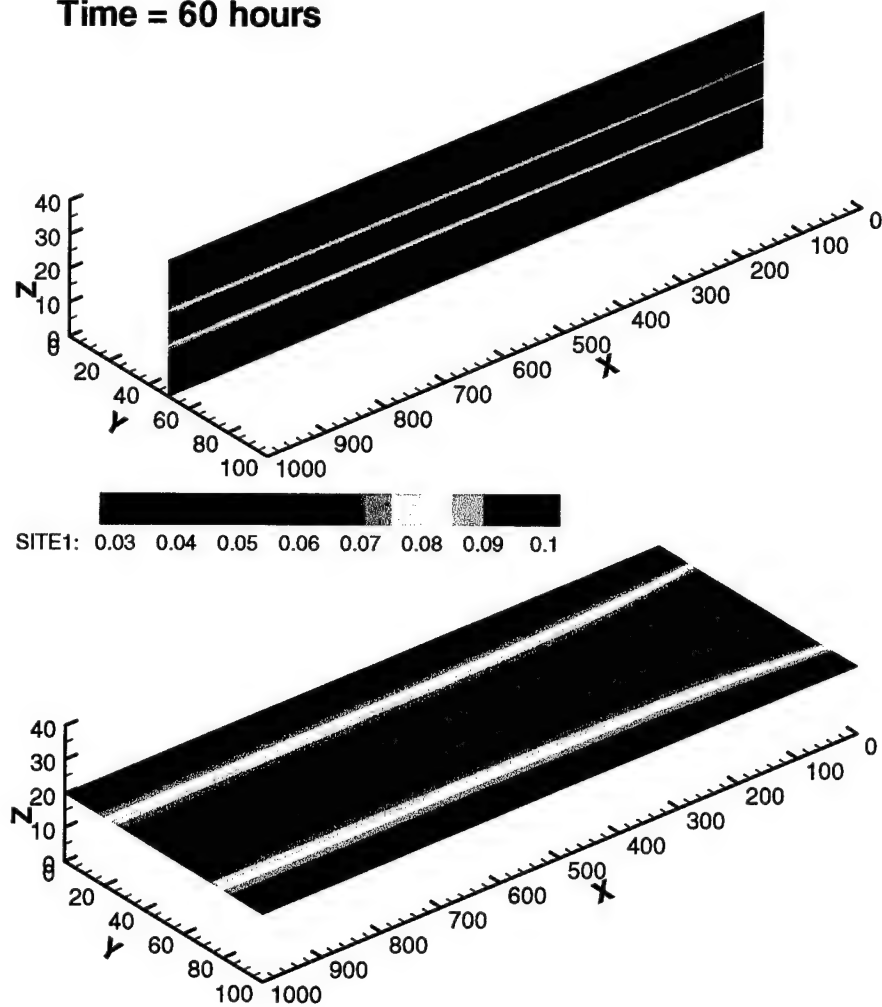


Figure 4.61. The concentration distribution of the 1st adsorbing site [g/m³] at time = 60 hour in the 3-D transport example.

Time = 60 hours

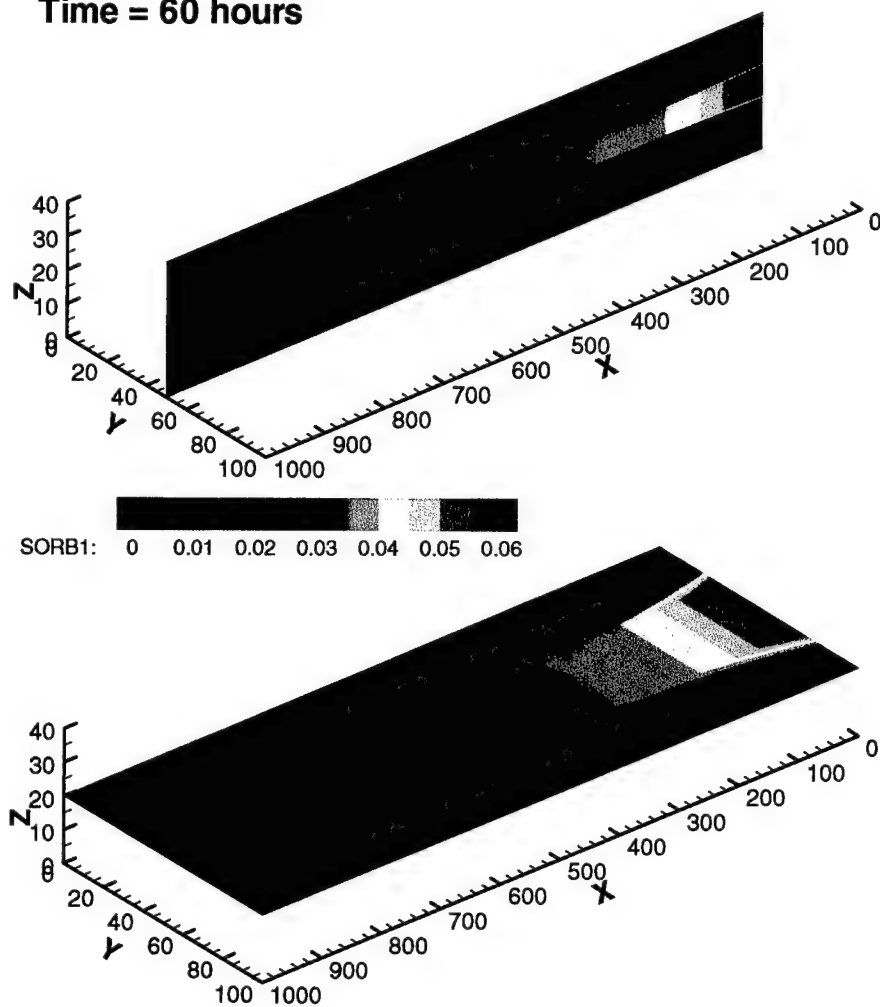


Figure 4.62. The concentration distribution of the 1st adsorbed chemical [g/m³] at time = 60 hour in the 3-D transport example.

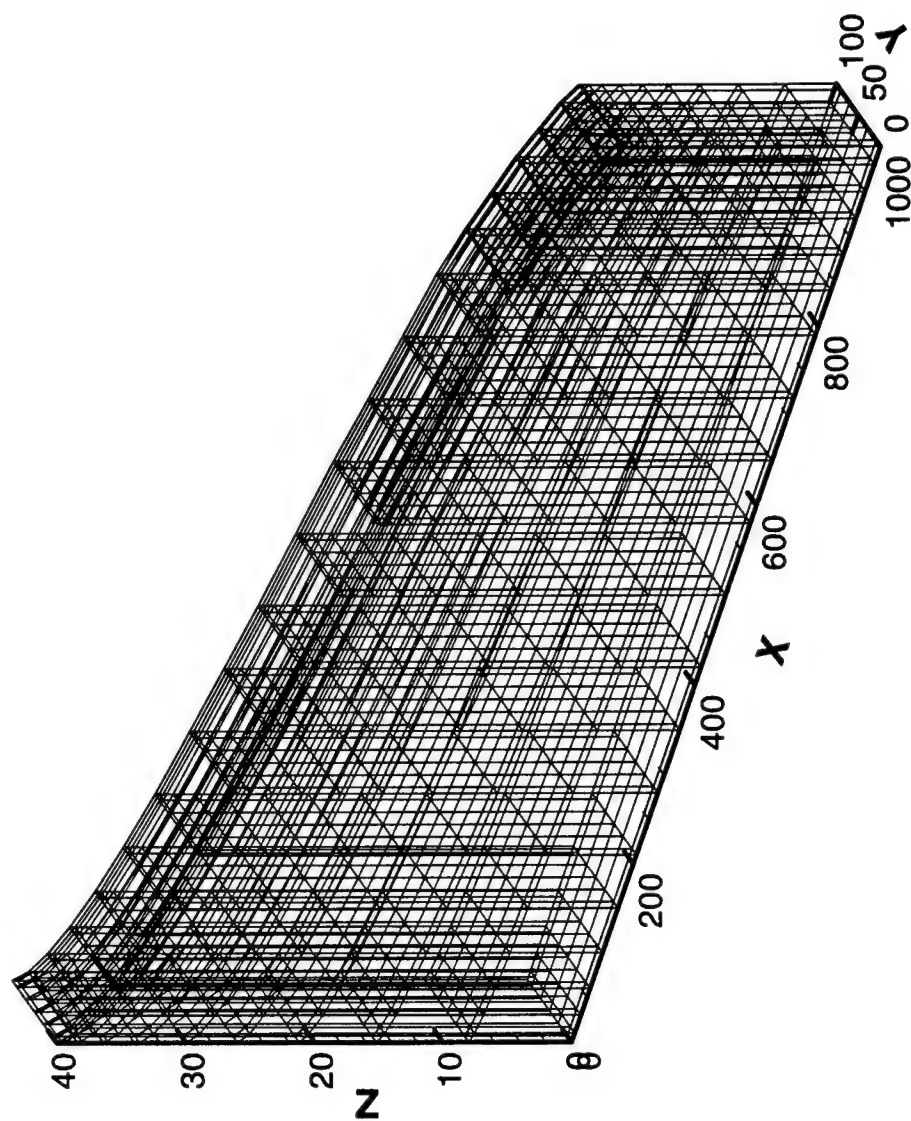
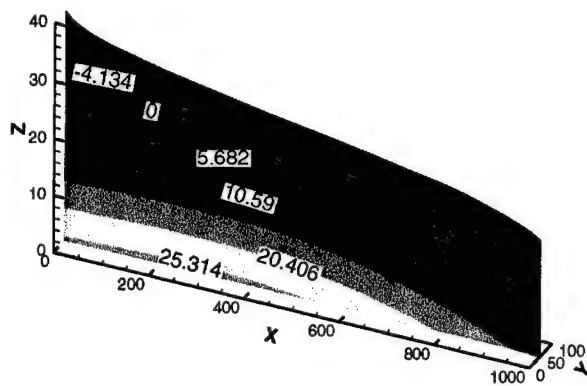
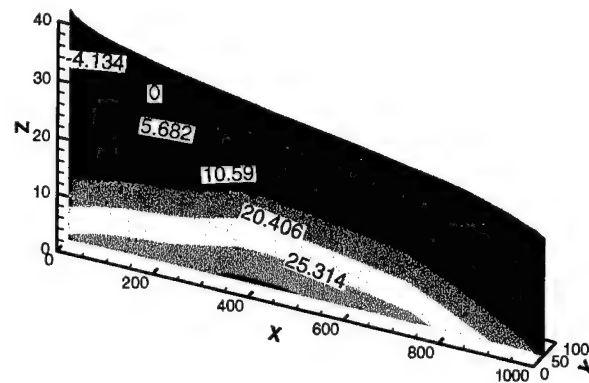


Figure 4.63. The domain and discretization of the 3-D flow and transport example.

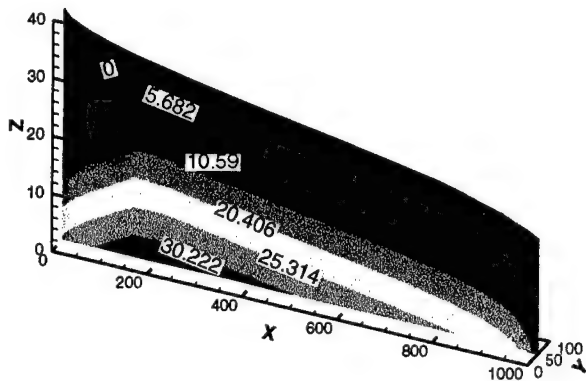
Time = 0 hour



Time = 40 minutes



Time = 1 hour 35 minutes



Time = 6 hours

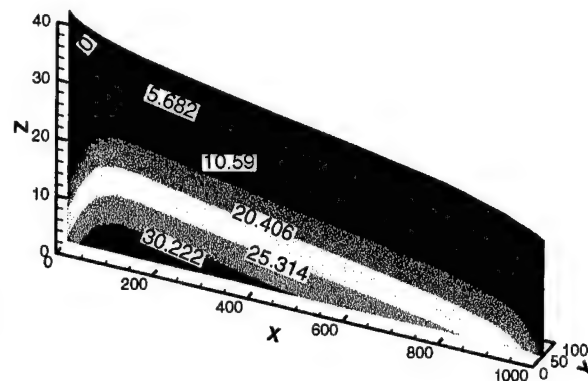


Figure 4.64. The pressure head distribution at various times for the 3-D flow and transport example.

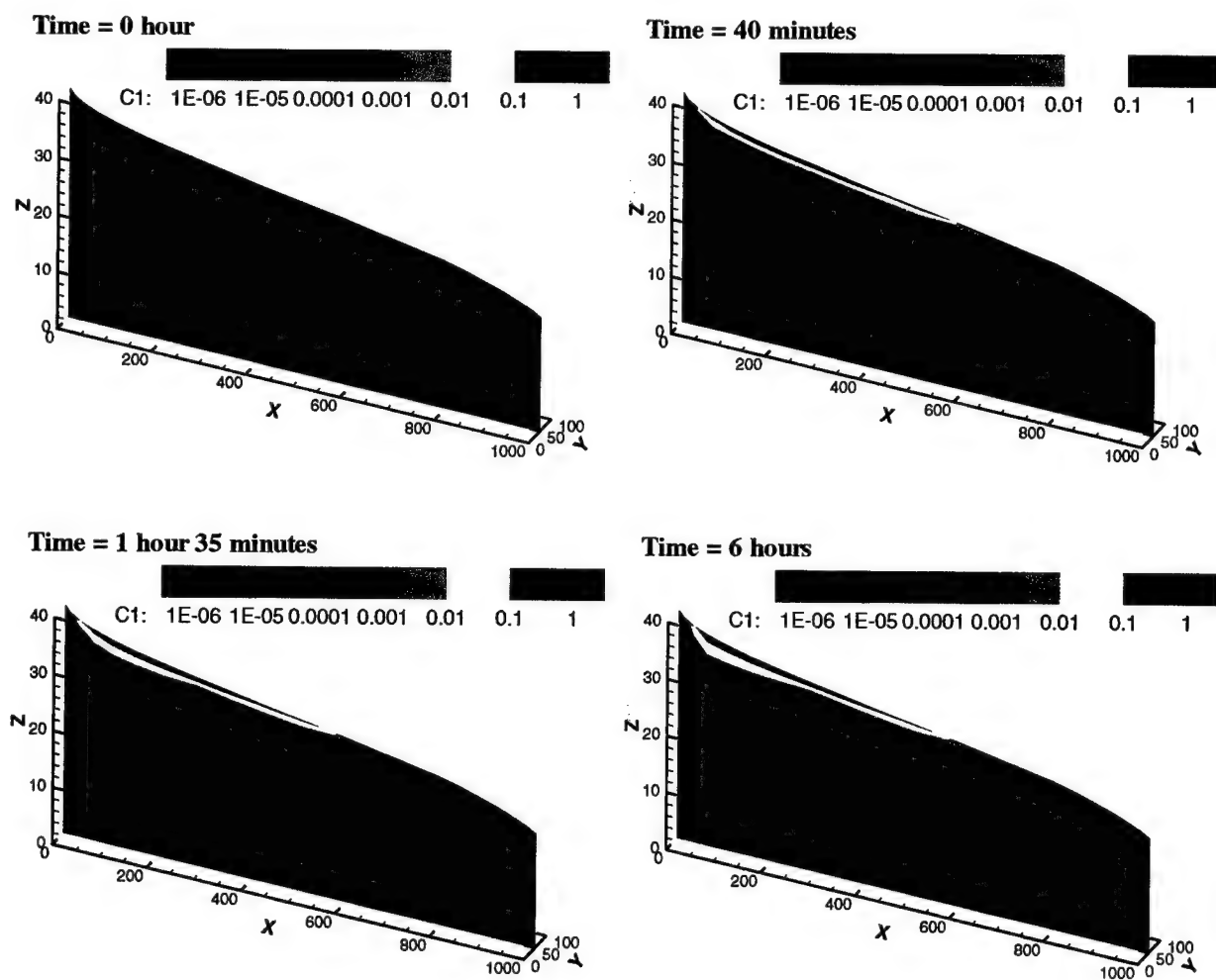


Figure 4.65. The concentration distribution of the 1st (or the 2nd) dissolved chemical [g/m³] at various times for the 3-D flow and transport example.

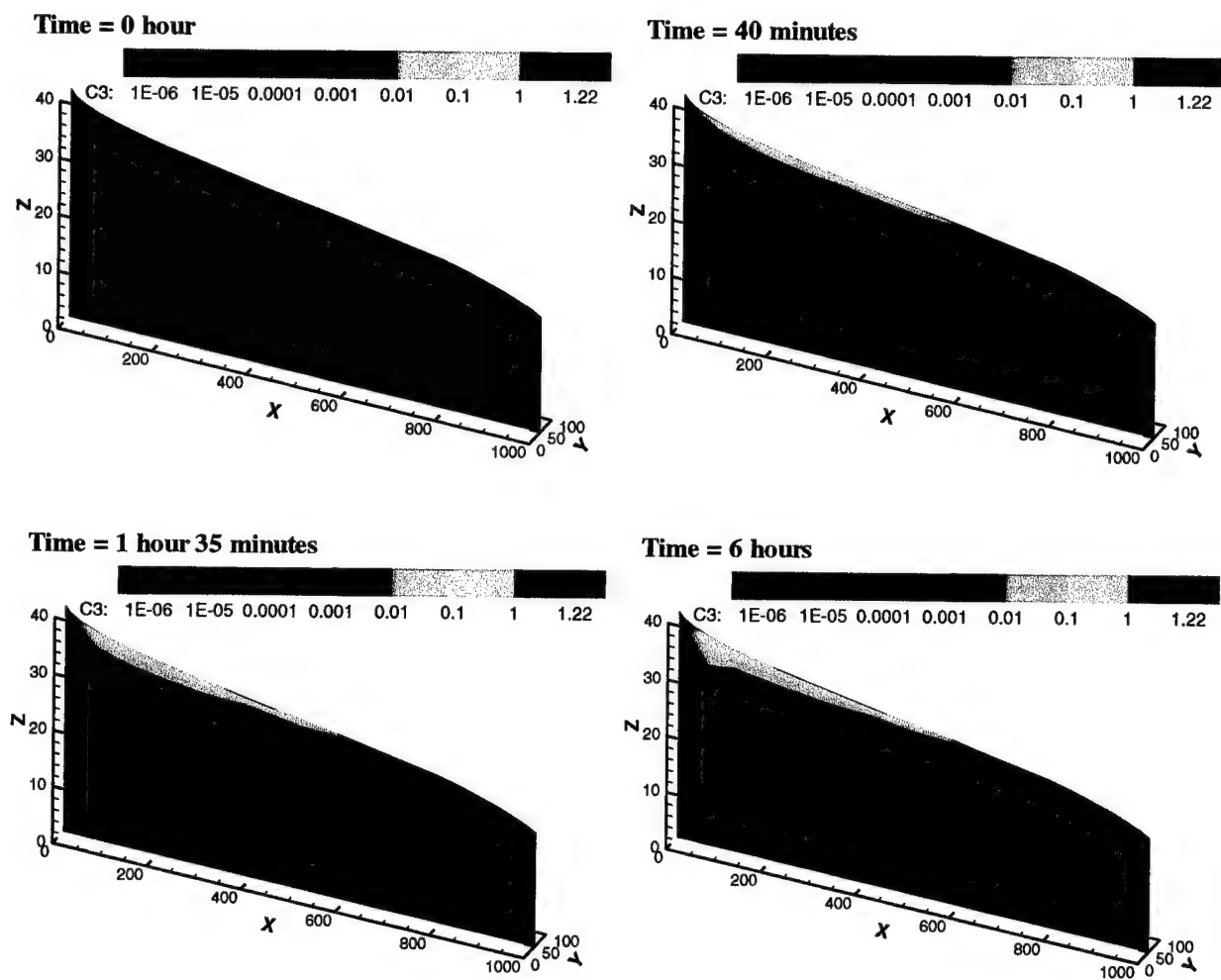
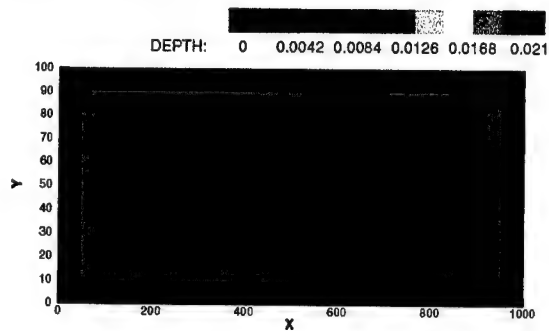
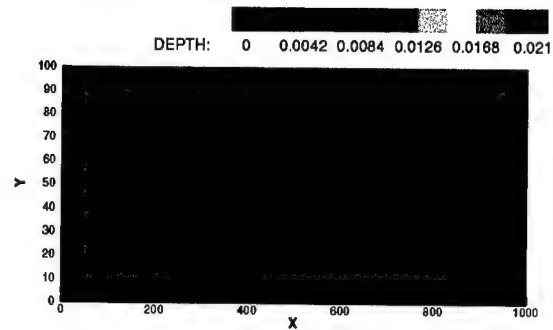


Figure 4.66. The concentration distribution of the 3rd dissolved chemical [g/m^3] at various times for the 3-D flow and transport example.

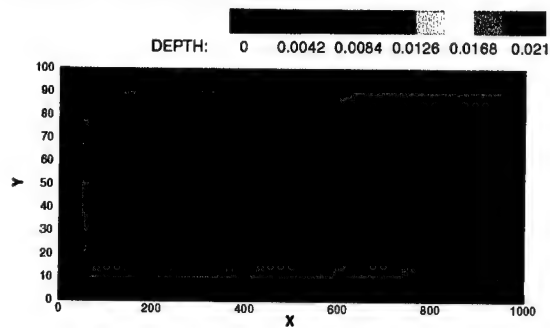
Time = 0 hour



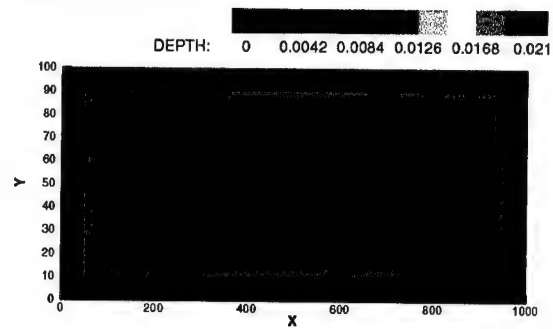
Time = 20 minutes



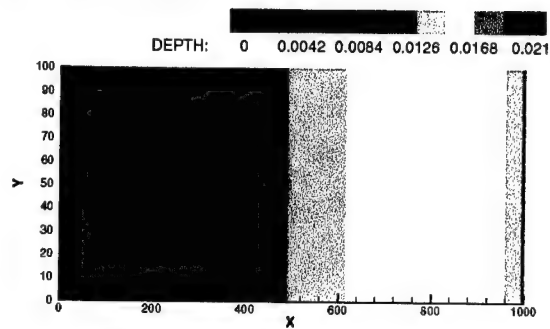
Time = 1 hour 20 minutes



Time = 2 hours



Time = 3 hours



Time = 6 hours

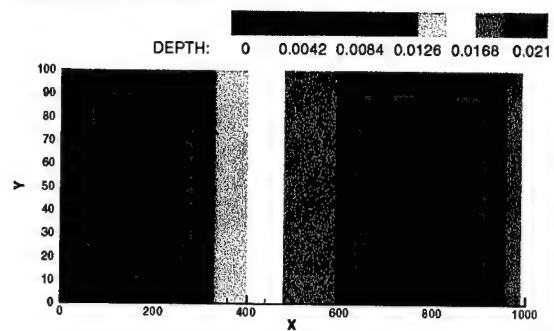
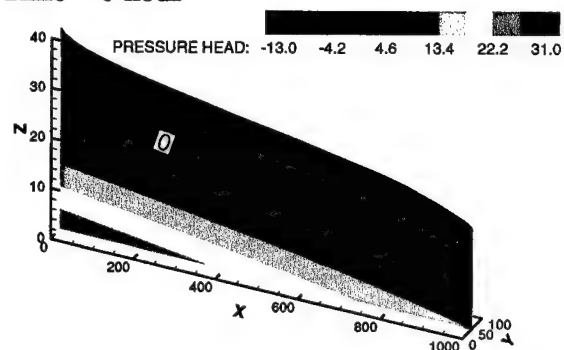
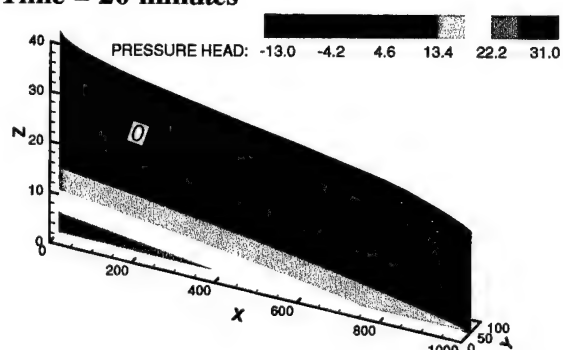


Figure 4.67. The overland water depth distribution at various times for the 2-D/3-D flow example.

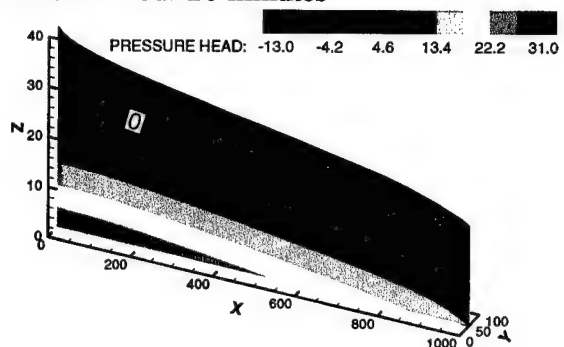
Time = 0 hour



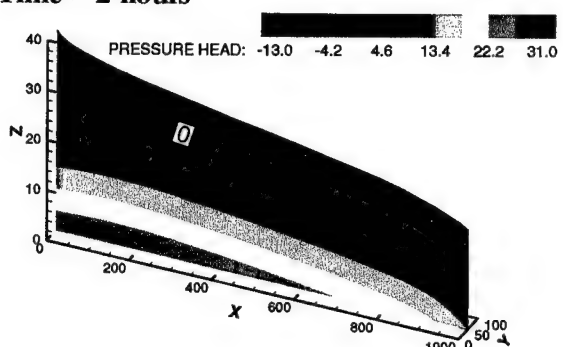
Time = 20 minutes



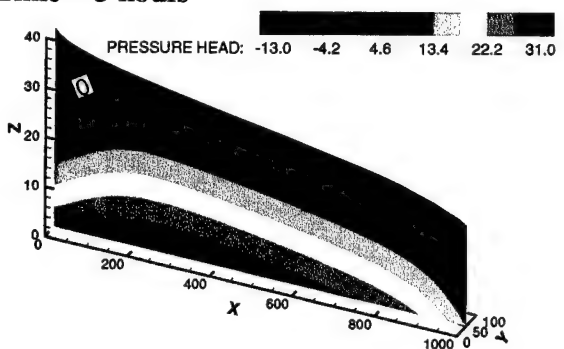
Time = 1 hour 20 minutes



Time = 2 hours



Time = 3 hours



Time = 6 hour

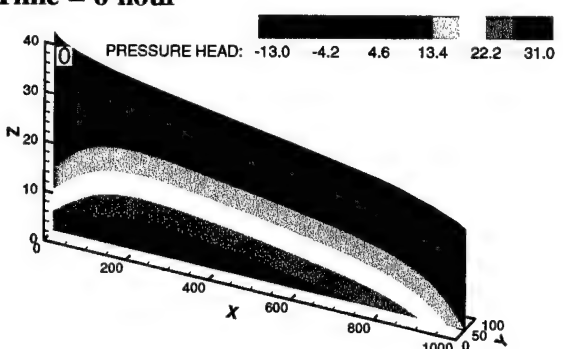
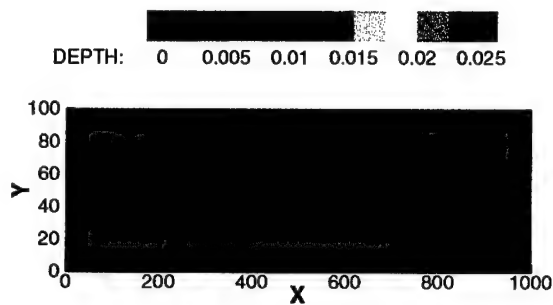
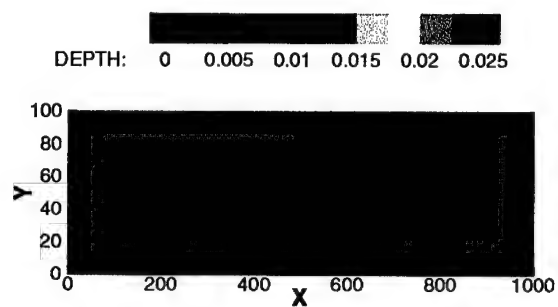


Figure 4.68. The pressure head distribution on the plane of $y = 50$ m at various times for the 2-D/3-D flow example.

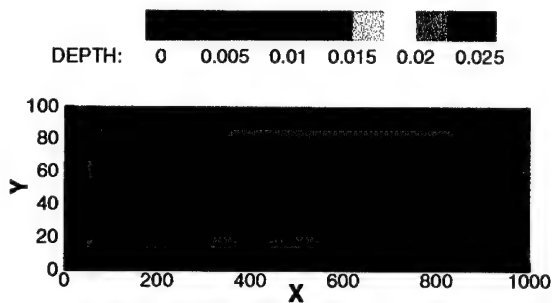
Time = 0 hour



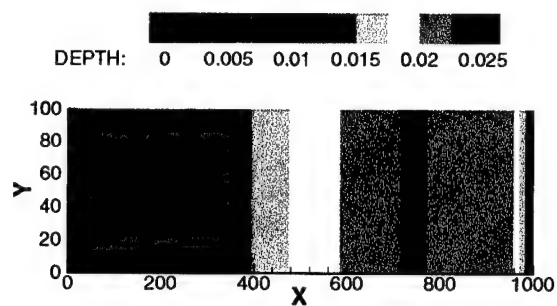
Time = 1 hour



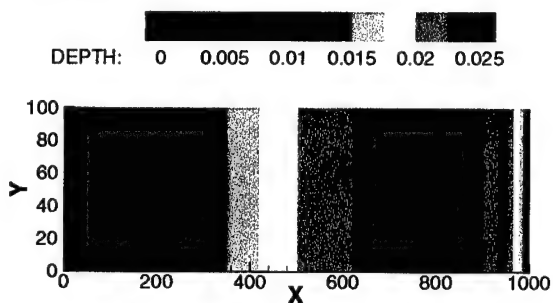
Time = 2 hours



Time = 3 hours



Time = 4 hours



Time = 6 hours

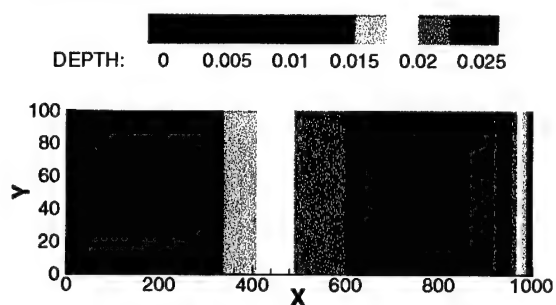
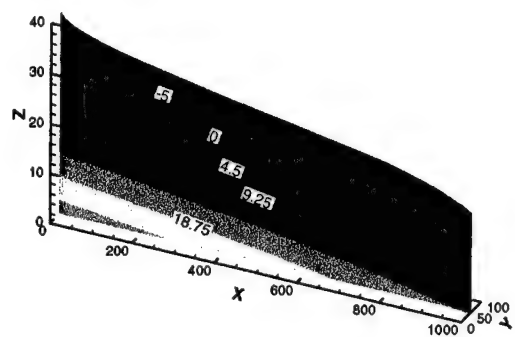
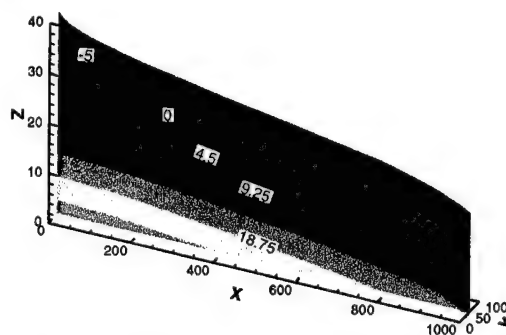


Figure 4.69. The overland water depth distribution at various times for the 2-D/3-D flow and transport example.

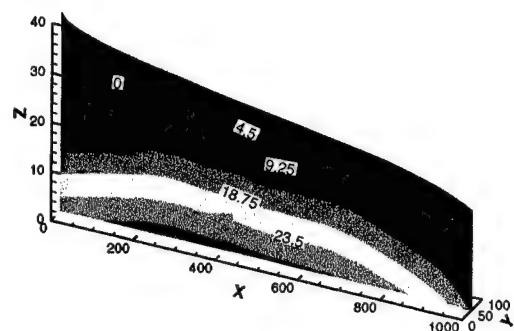
Time = 0 hour



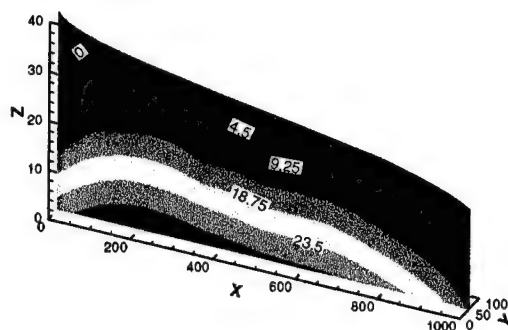
Time = 1 hour



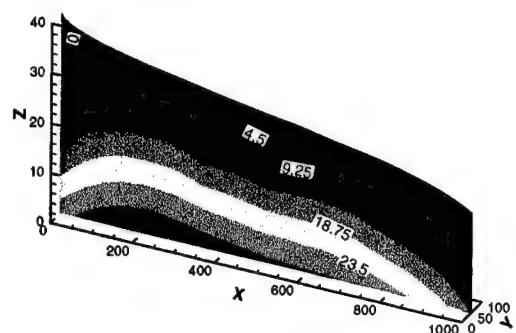
Time = 2 hours



Time = 3 hours



Time = 4 hours



Time = 6 hours

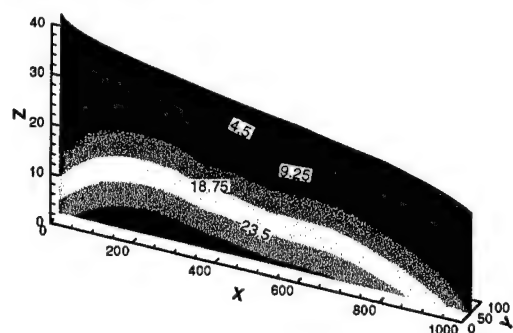
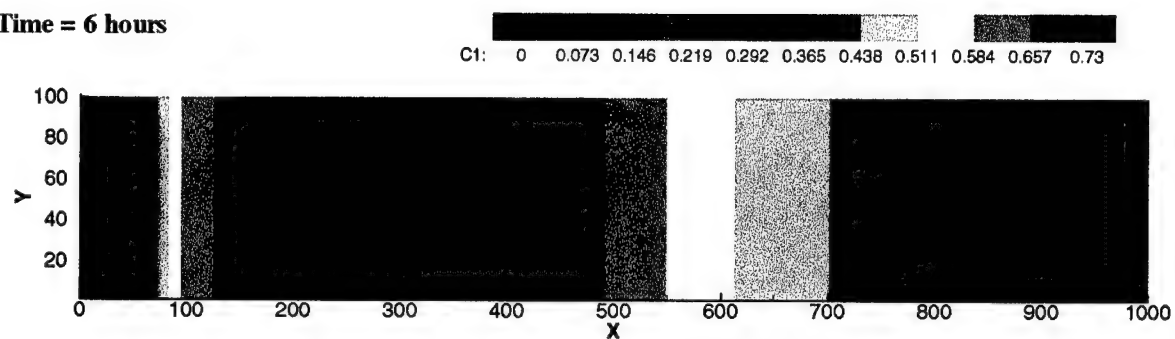
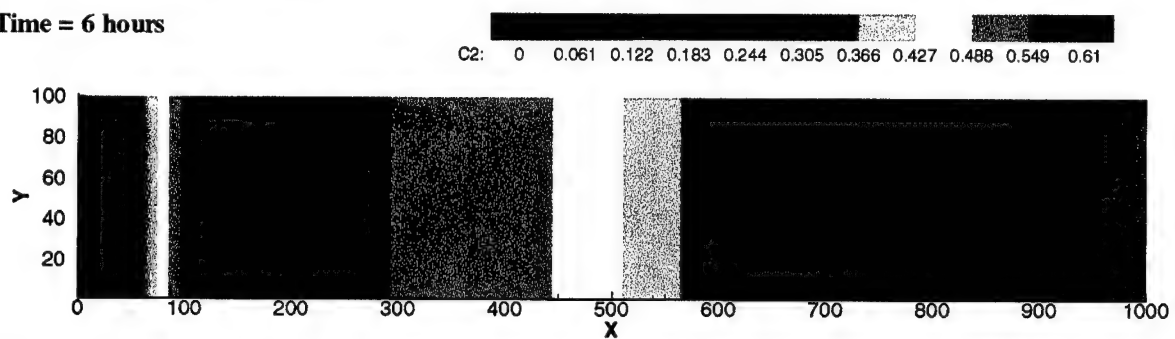


Figure 4.70. The pressure head distribution on the plane of $y = 50$ m at various times for the 2-D/3-D flow and transport example.

Time = 6 hours



Time = 6 hours



Time = 6 hours

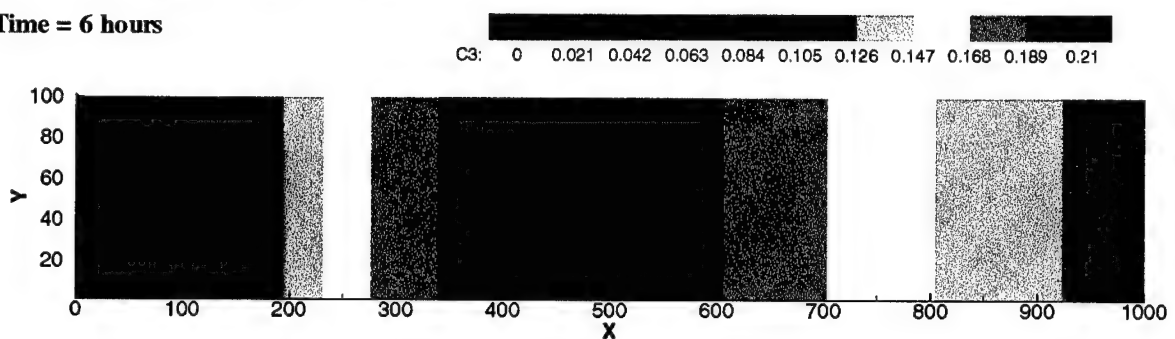
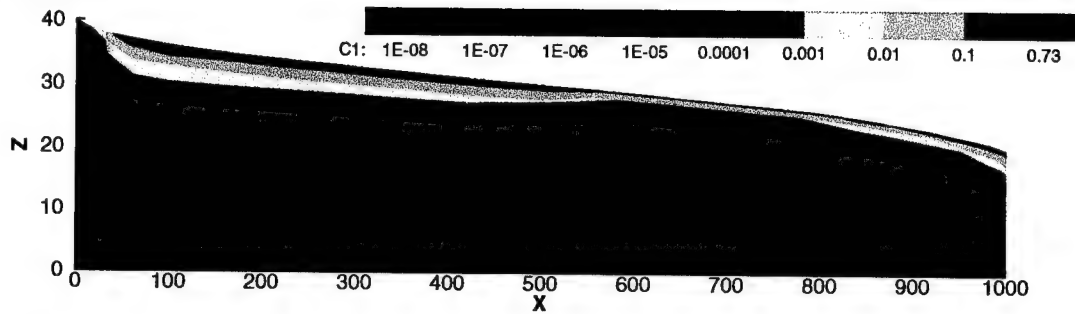
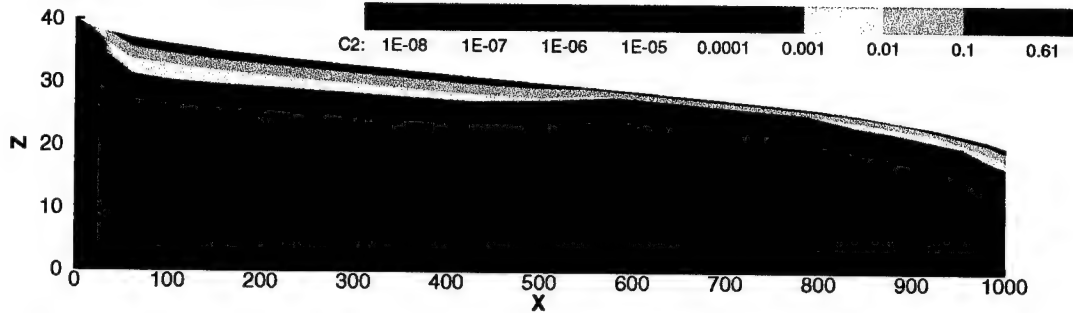


Figure 4.71. The concentration distribution of dissolved chemicals [g/m^3] on 2-D overland at time = 6 hours for the 2-D/3-D flow and transport example.

Time = 6 hours



Time = 6 hours



Time = 6 hours

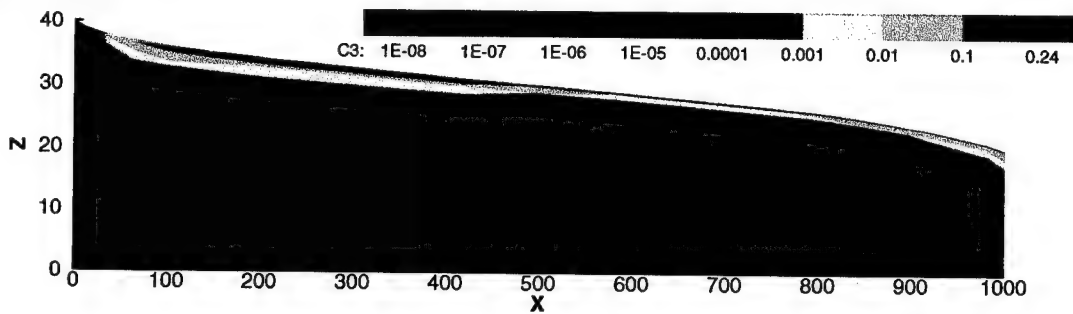


Figure 4.72. The concentration distribution of dissolved chemicals [g/m³] on the y = 50 m vertical plane of 3-D subsurface at time = 6 hours for the 2-D/3-D flow and transport example.

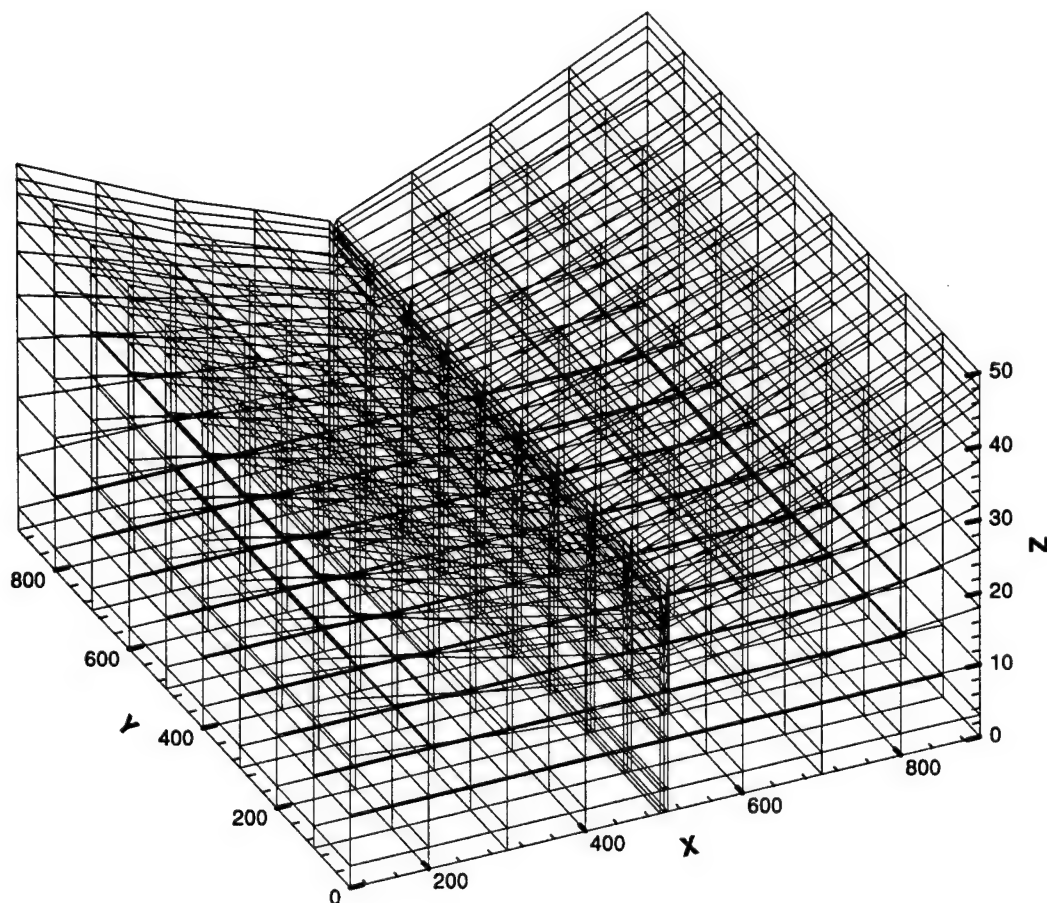


Figure 4.73. The discretization of the 1-D/2-D/3-D flow example.

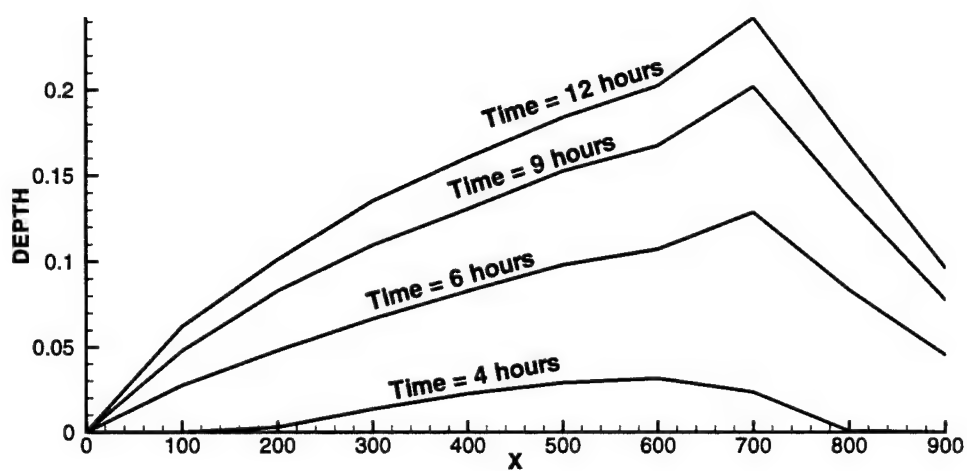


Figure 4.74. The river/stream water depth at various times for the 1-D/2-D/3-D flow example.

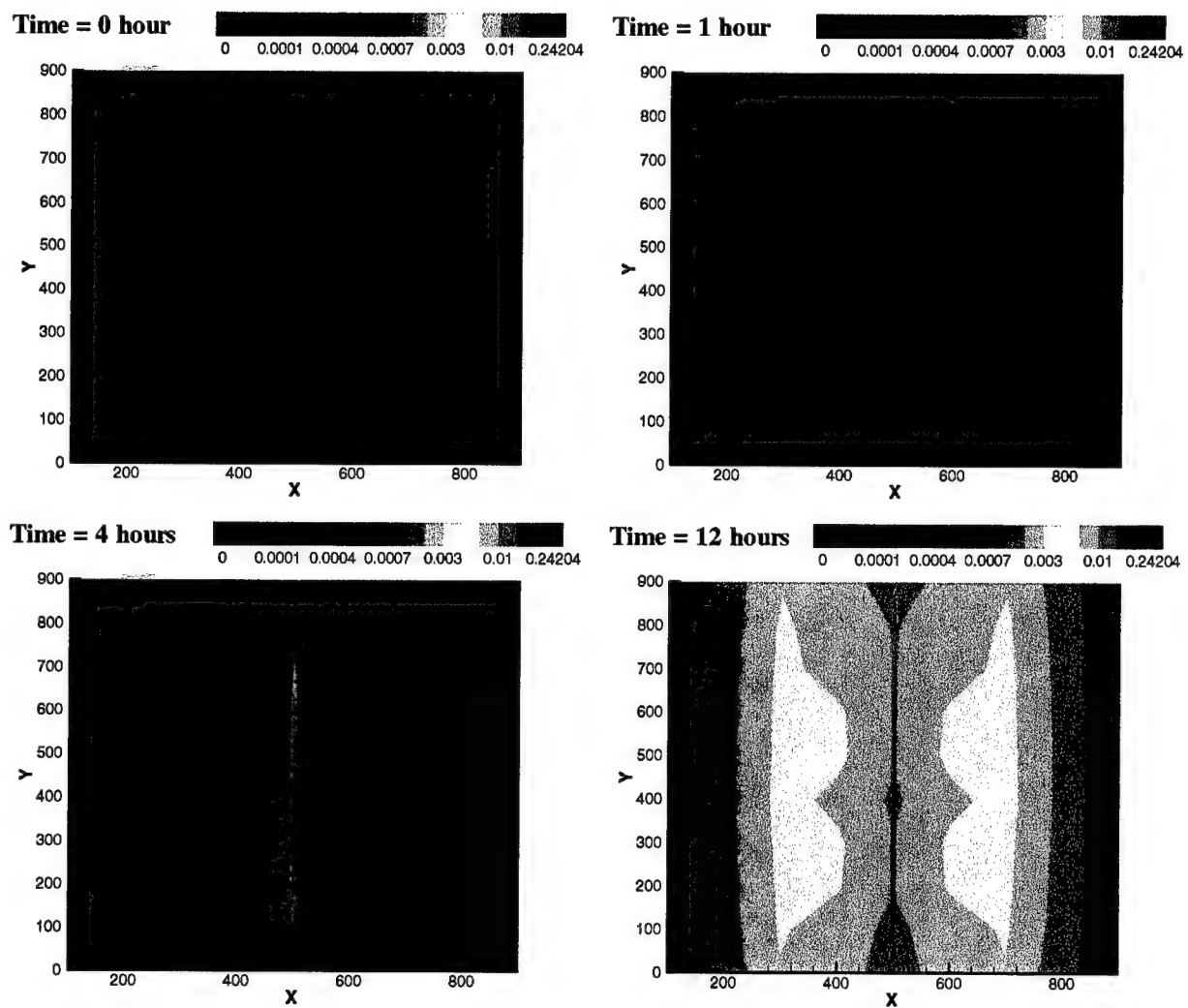
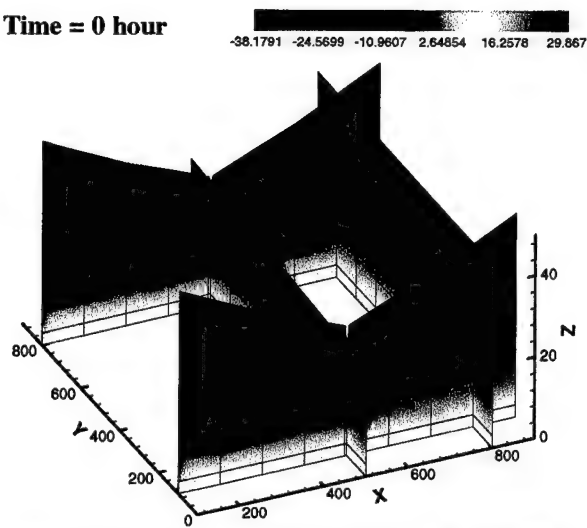
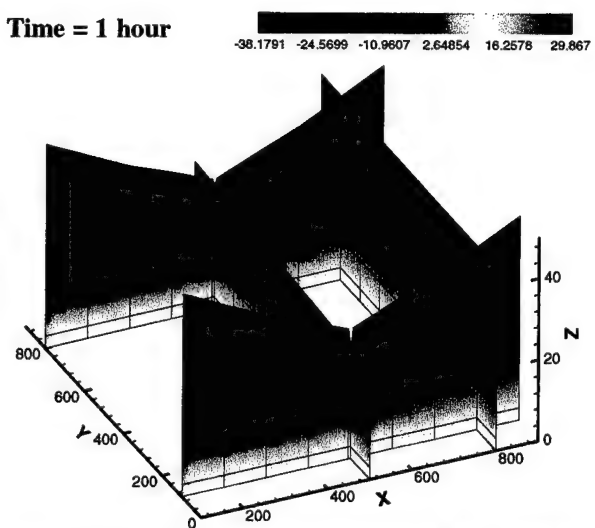


Figure 4.75. The overland water depth at various times for the 1-D/2-D/3-D flow example.

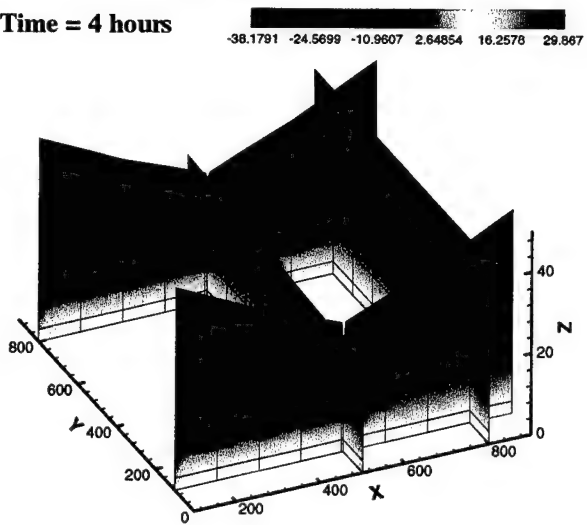
Time = 0 hour



Time = 1 hour



Time = 4 hours



Time = 12 hours

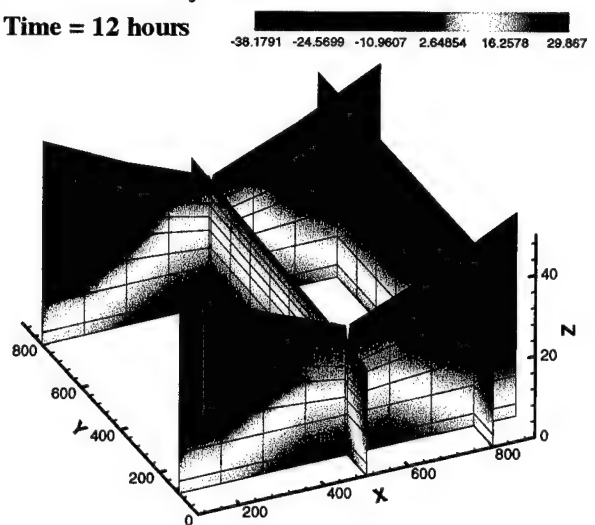
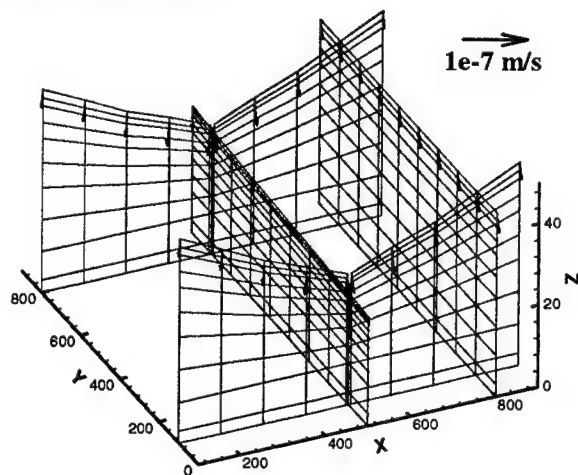
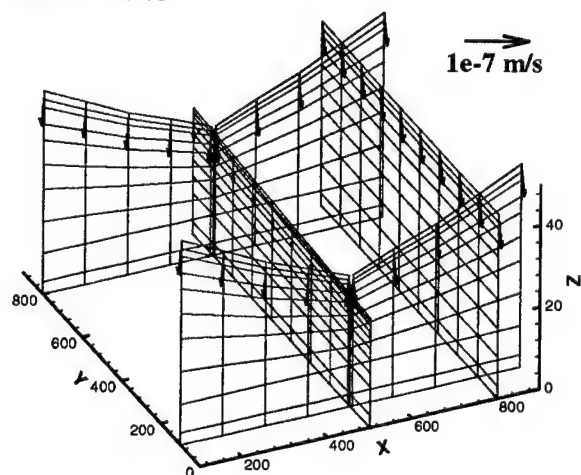


Figure 4.76. The pressure head distribution on four vertical planes at various times for the 1-D/2-D/3-D flow example.

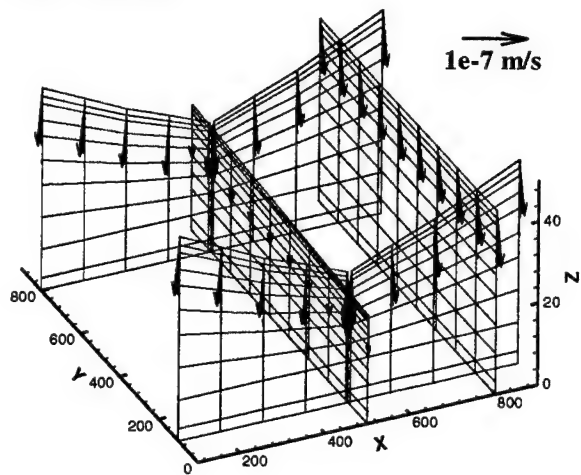
Time = 20 minutes



Time = 1 hour



Time = 4 hours



Time = 12 hours

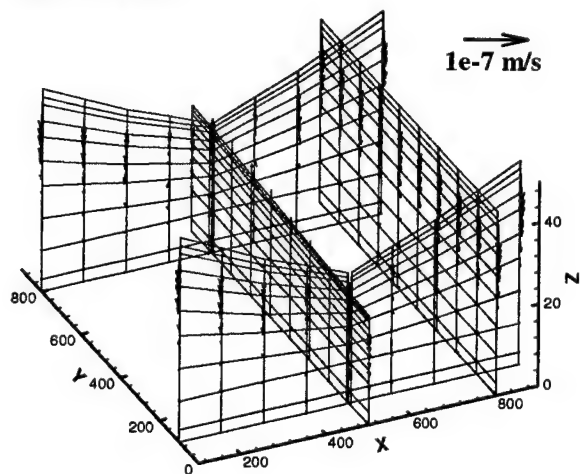


Figure 4.77. The Darcy velocity (specific discharge) on four vertical planes at various times for the 1-D/2-D/3-D flow example.

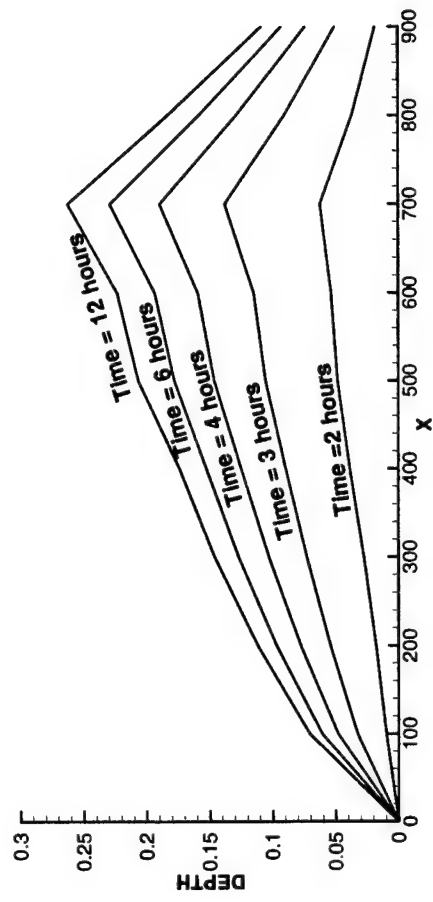


Figure 4.78. The river/stream water depth at various times for the 1-D/2-D/3-D flow and transport example.

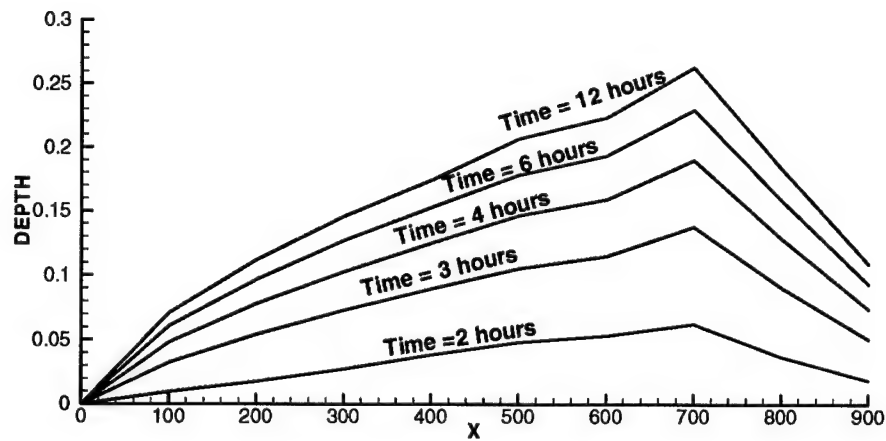


Figure 4.78. The river/stream water depth at various times for the 1-D/2-D/3-D flow and transport example.

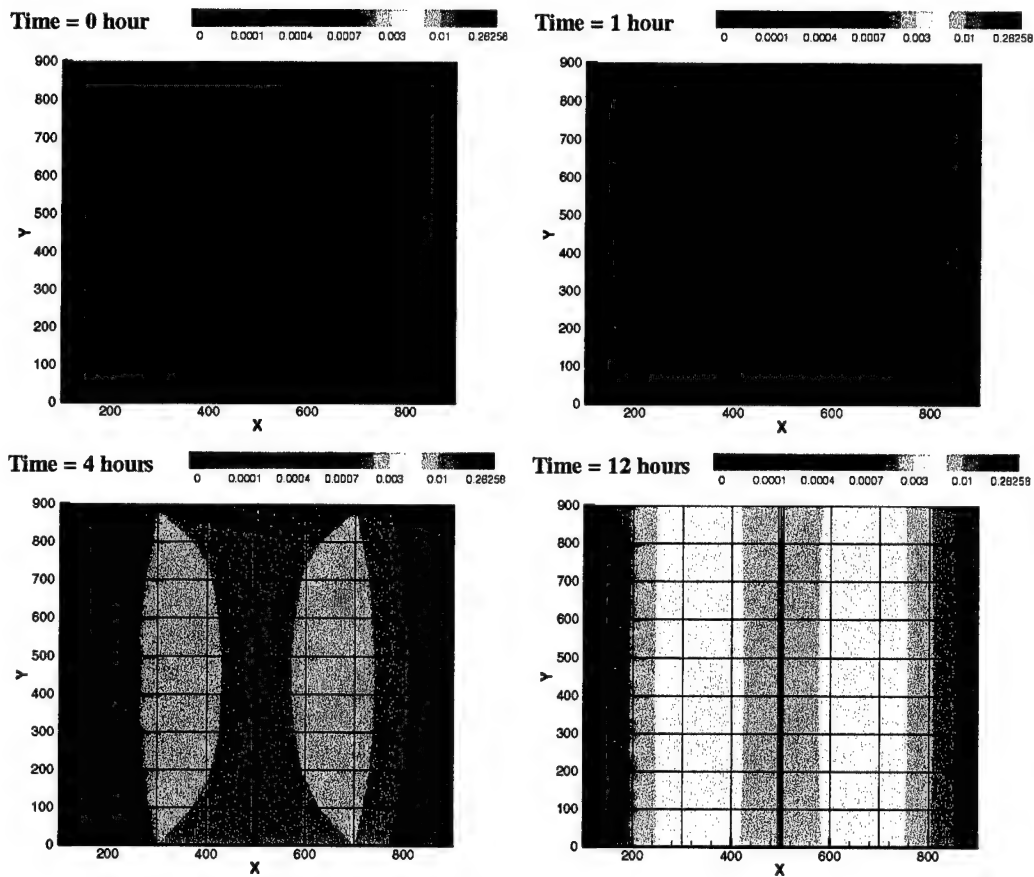
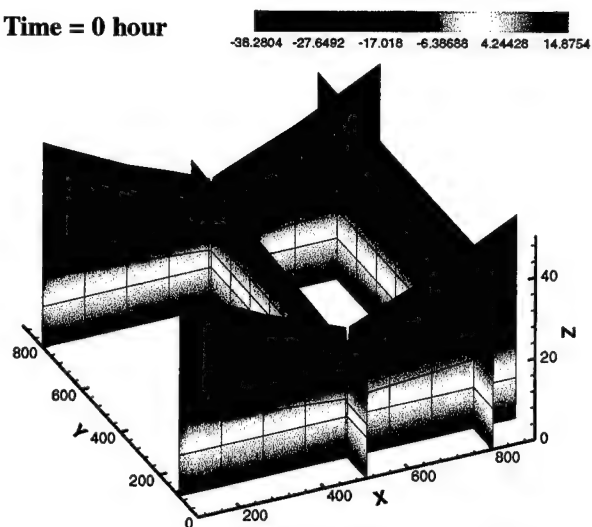
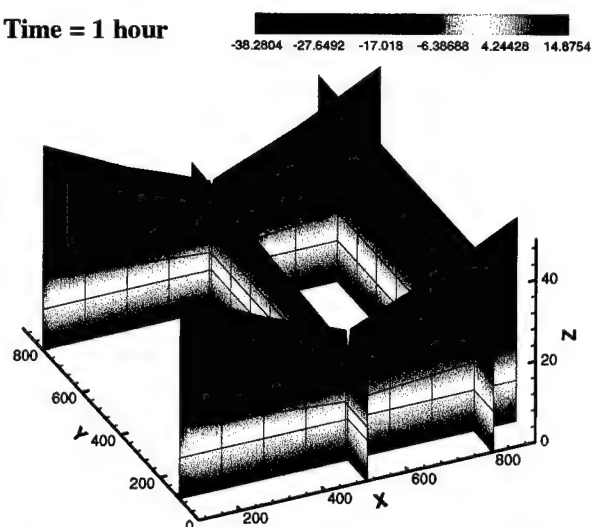


Figure 4.79. The overland water depth at various times for the 1-D/2-D/3-D flow and transport example.

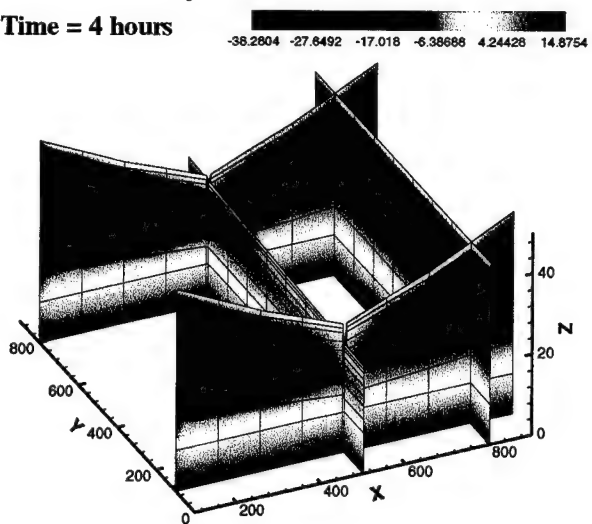
Time = 0 hour



Time = 1 hour



Time = 4 hours



Time = 12 hours

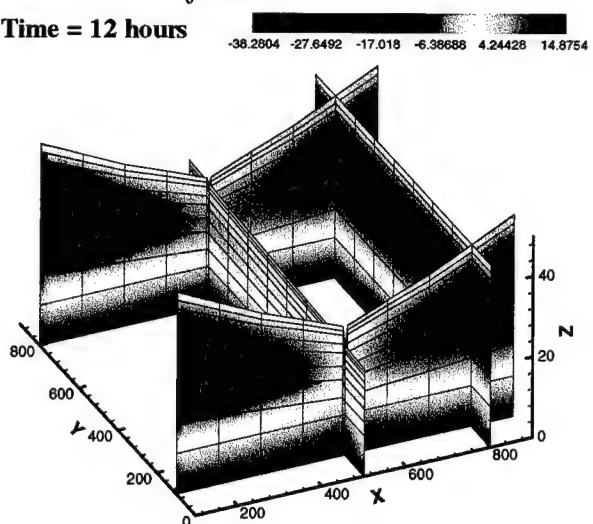


Figure 4.80. The pressure head distribution at various times for the 1-D/2-D/3-D flow and transport example.

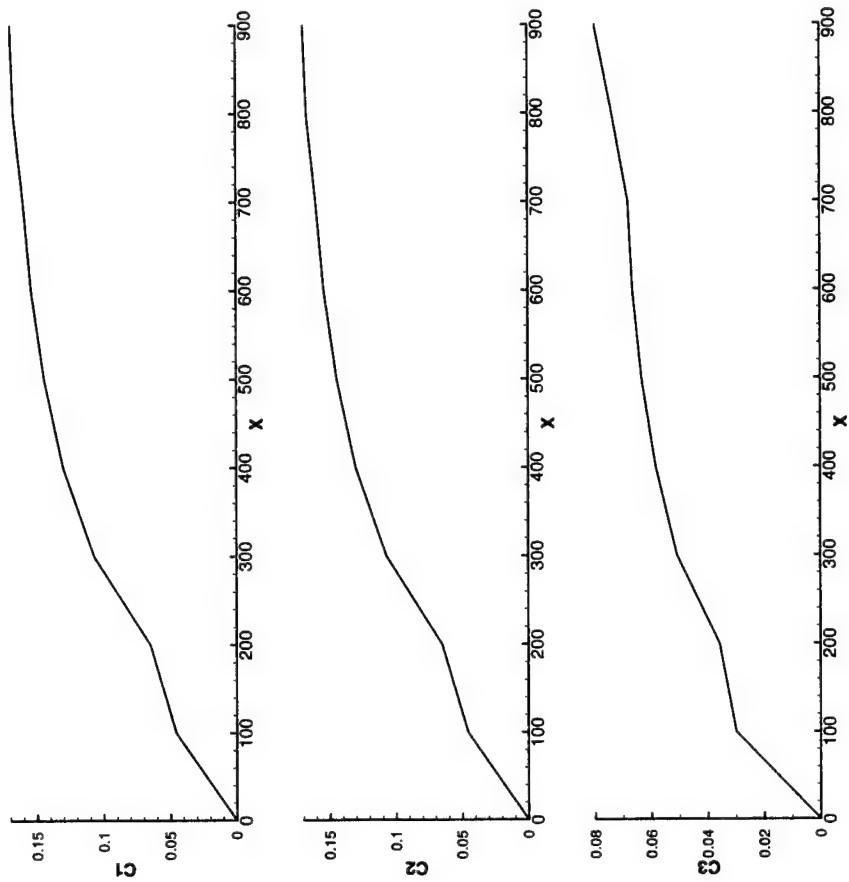


Figure 4.81. The concentration distribution of dissolved chemicals [g/m³] in river/stream at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

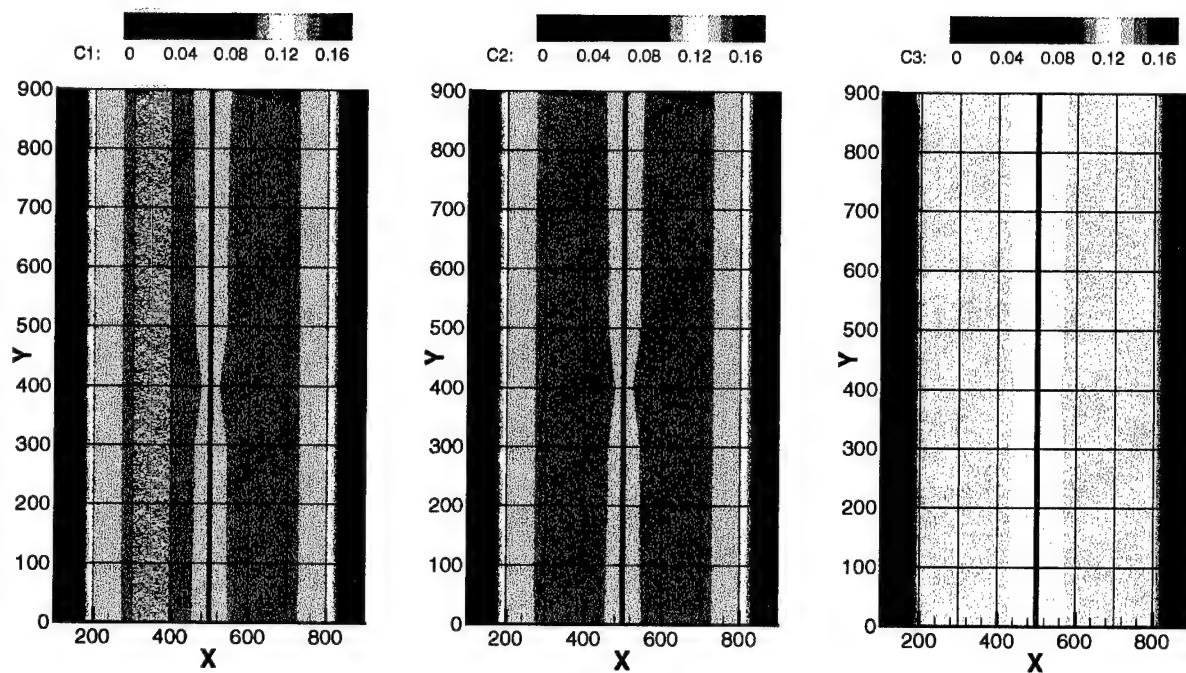


Figure 4.82. The concentration distribution of dissolved chemicals [g/m³] on overland at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

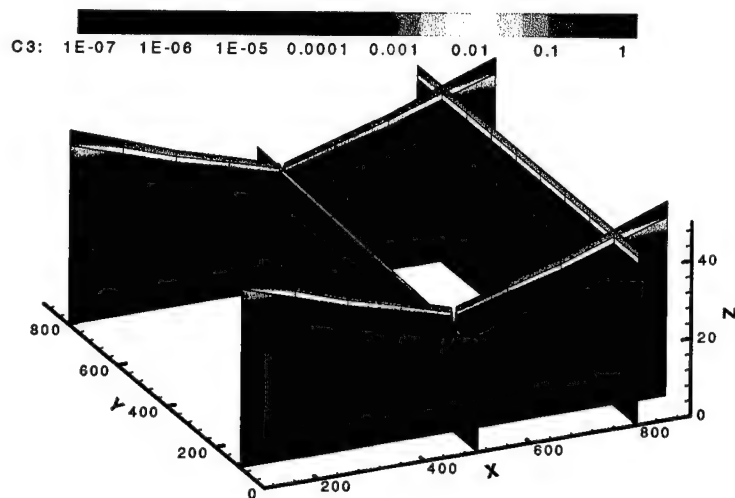
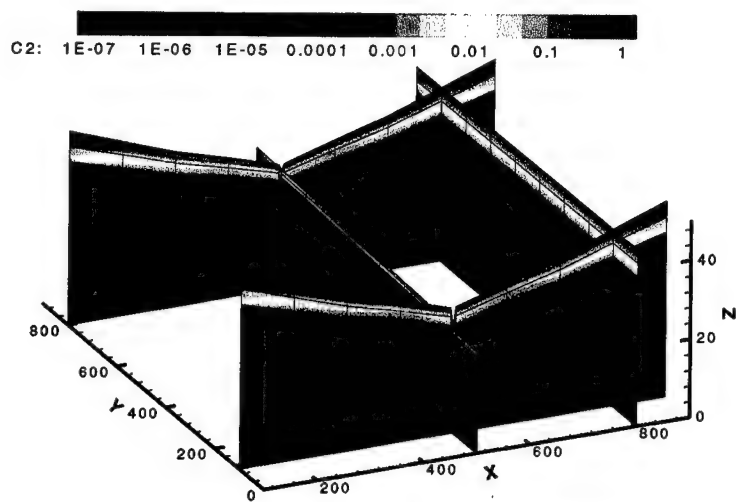
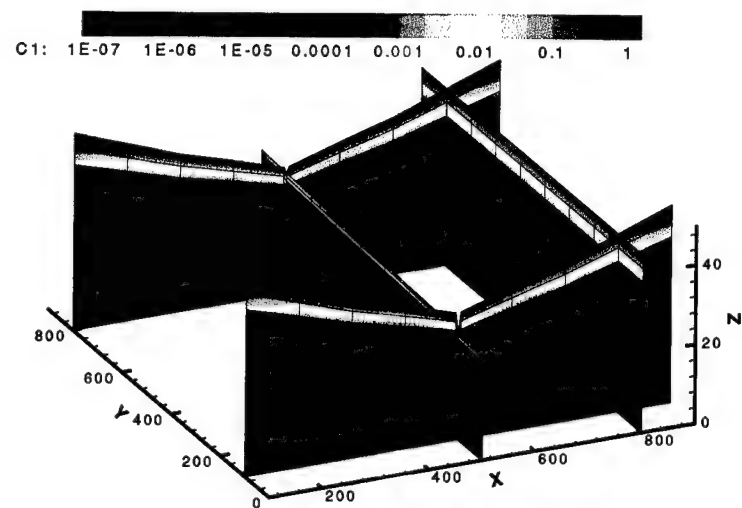


Figure 4.83. The concentration distribution of dissolved chemicals [g/m^3] in the subsurface at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

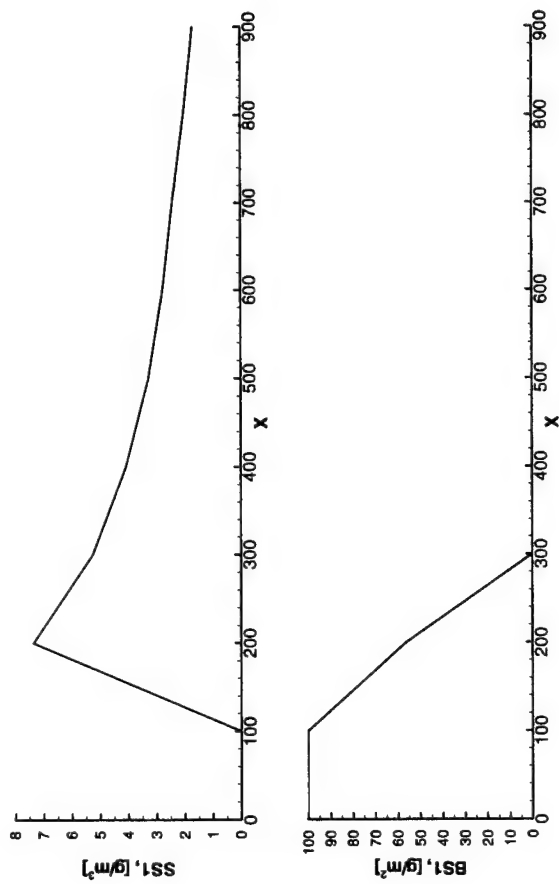


Figure 4.84. The concentration distribution of sediments in river/stream at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

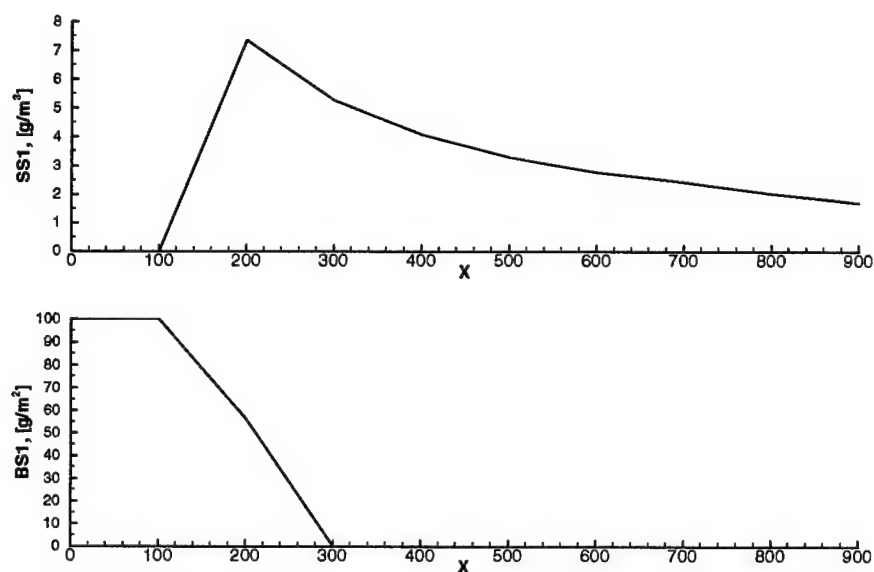


Figure 4.84. The concentration distribution of sediments in river/stream at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

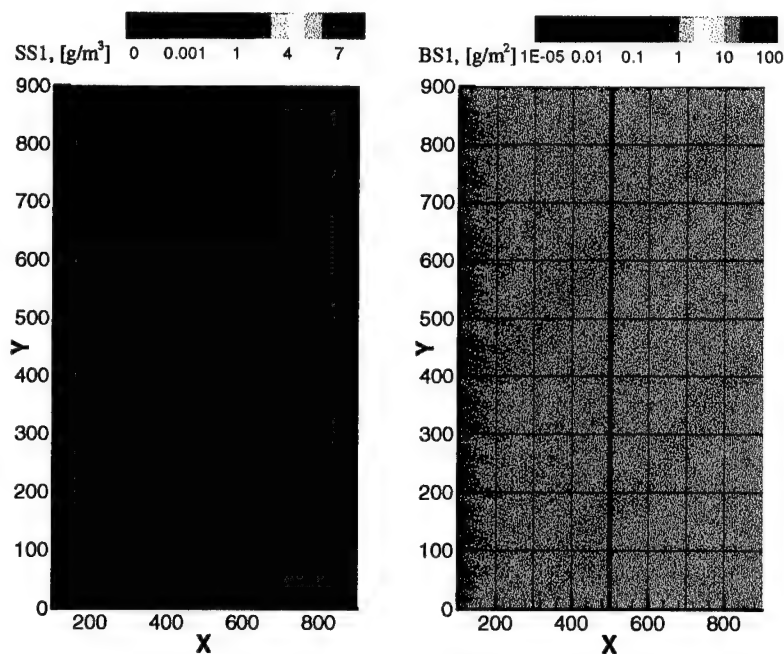


Figure 4.85. The concentration distribution of sediments on overland at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

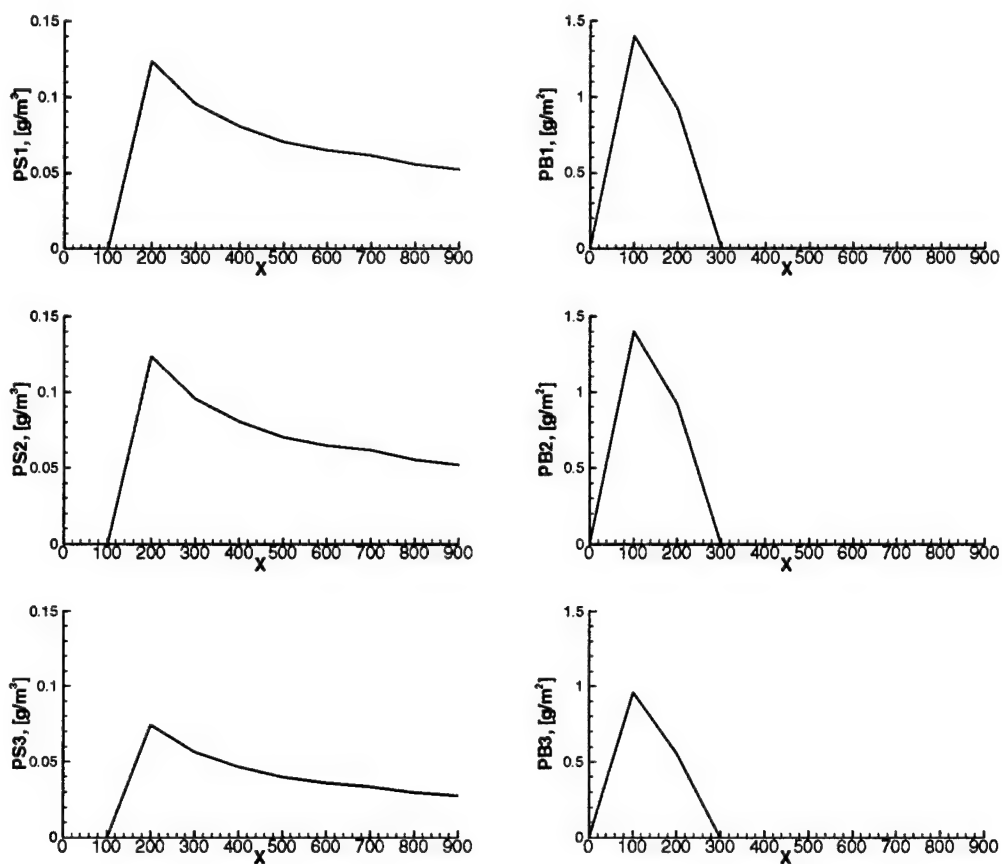


Figure 4.86. The concentration distribution of particulate chemicals in river/stream at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

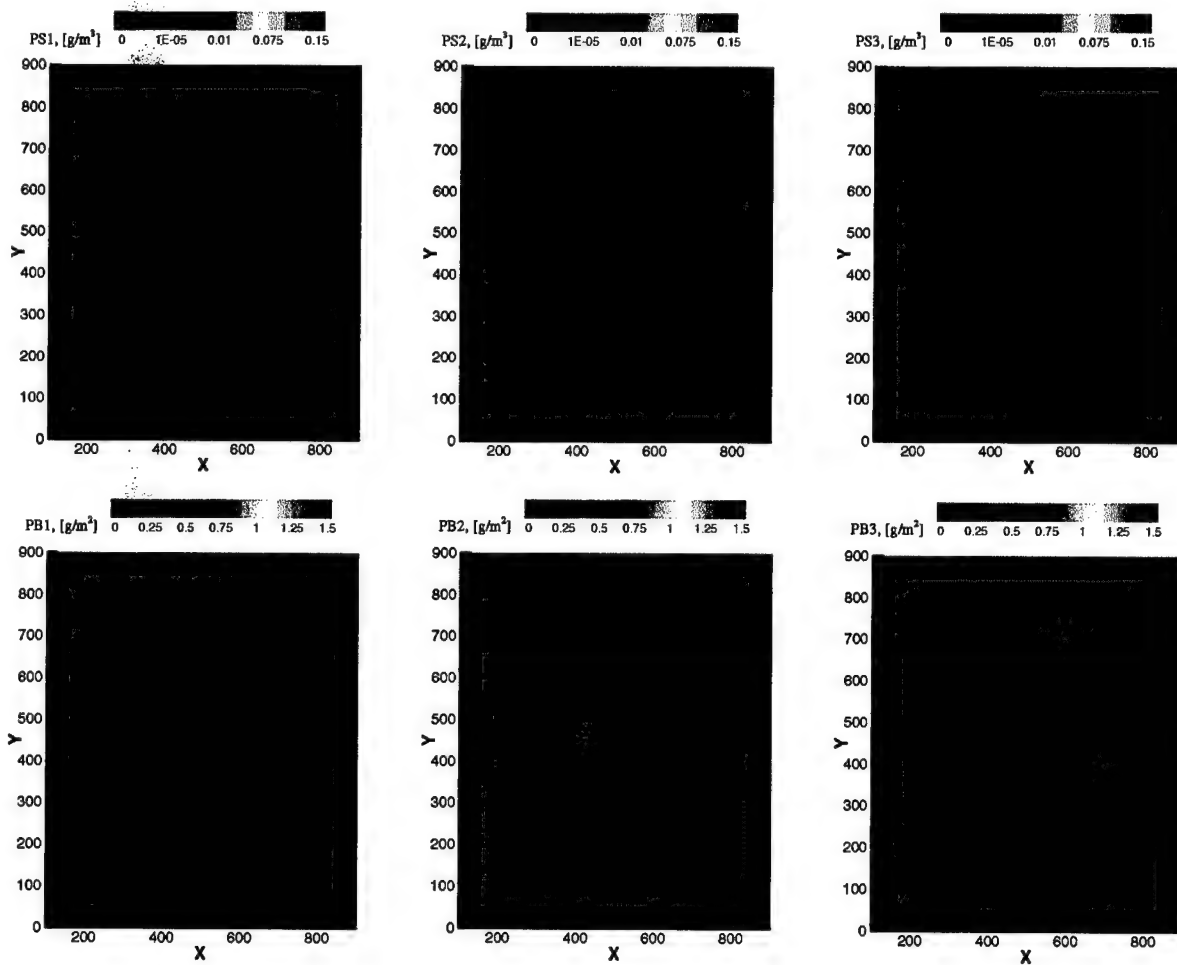
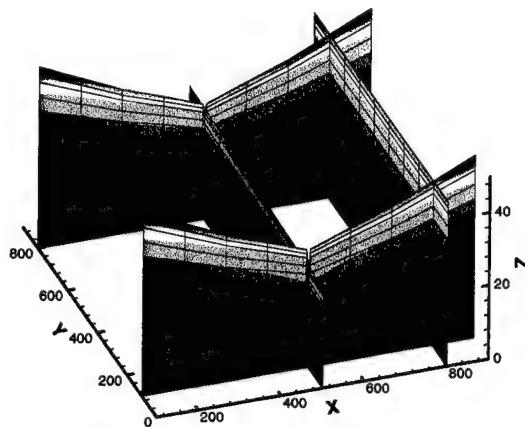
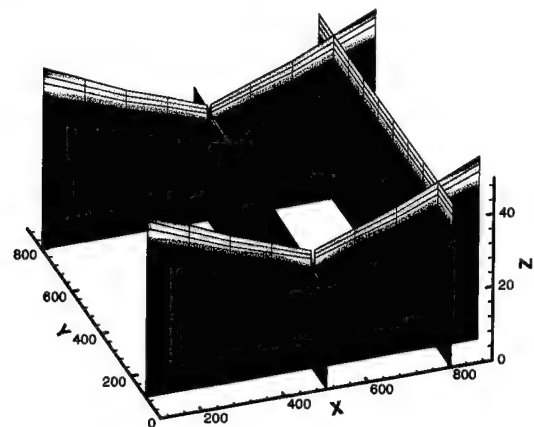


Figure 4.87. The concentration distribution of particulate chemicals on overland at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

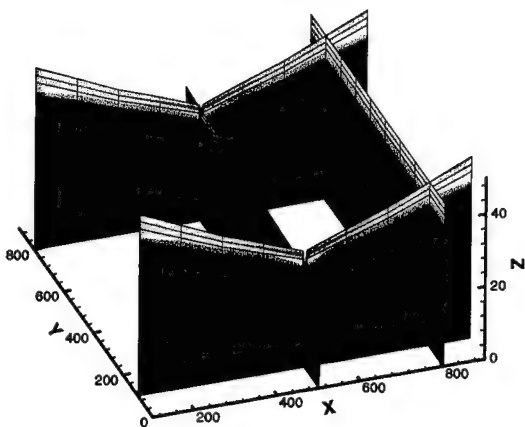
SITE1: 1E-05 0.0001 0.001 0.01 0.1 1 2



SORB1: 1E-05 0.0001 0.001 0.01 0.1 0.392



SORB2: 1E-05 0.0001 0.001 0.01 0.1 0.8286



SORB3: 1E-05 0.0001 0.001 0.01 0.1 1 1.8112

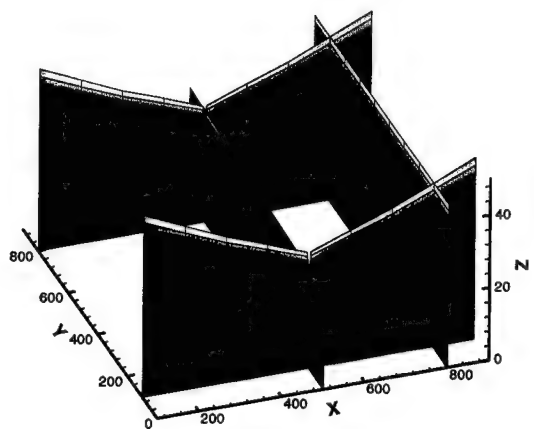


Figure 4.88. The concentration distribution of the adsorbing site and adsorbed chemicals [g/m³] in the subsurface at Time = 12 hours for the 1-D/2-D/3-D flow and transport example.

Appendix I. DATA INPUT GUIDE

This data input guide is composed of eleven files: three for 3-D subsurface flow/transport, three for 2-D overland flow/transport, three for 1-D river/stream flow/transport, one for chemical/sediment information and one for 1-D/2-D/3-D mapping. They are described as follows.

I.1. File 1: 3-D subsurface geometry file (.3dm)

<u>Value</u>	<u>Description</u>
WMS3DM	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>GE Card</u>		<u>Mesh card</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GE	Card group identifier
C 3	IC3	8	Hexahedral element. One entry for each hexahedral element in the mesh.
1	M	+	id of global element.
2	IE(M,1)	+	id of the global node that serves as the 1 st element node of the global element.
3	IE(M,2)	+	id of the global node that serves as the 2 nd element node of the global element.
4	IE(M,3)	+	id of the global node that serves as the 3 rd element node of the global element.
5	IE(M,4)	+	id of the global node that serves as the 4 th element node of the global element.
6	IE(M,5)	+	id of the global node that serves as the 5 th element node of the global element.
7	IE(M,6)	+	id of the global node that serves as the 6 th element node of the global element.
8	IE(M,7)	+	id of the global node that serves as the 7 th element node of the global element.
9	IE(M,8)	+	id of the global node that serves as the 8 th element node of the global element.
10	IE(M,9)	+	The material ID of this element.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GE	Card group identifier
C 3	IC3	6	Wedge or prism element. One entry for each wedge element in the mesh.
1	M	+	id of global element.
2	IE(M,1)	+	id of the global node that serves as the 1 st element node of the global element.
3	IE(M,2)	+	id of the global node that serves as the 2 nd element node of the global element.
4	IE(M,3)	+	id of the global node that serves as the 3 rd element node of the global element.

5	IE(M,4)	+	id of the global node that serves as the 4 th element node of the global element.
6	IE(M,5)	+	id of the global node that serves as the 5 th element node of the global element.
7	IE(M,6)	+	id of the global node that serves as the 6 th element node of the global element.
8	IE(M,9)	+	The material ID of this element.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GE	Card group identifier
C 3	IC3	4	Tetrahedral element. One entry for each tetrahedral element in the mesh.
1	M	+	id of global element.
2	IE(M,1)	+	id of the global node that serves as the 1 st element node of the global element.
3	IE(M,2)	+	id of the global node that serves as the 2 nd element node of the global element.
4	IE(M,3)	+	id of the global node that serves as the 3 rd element node of the global element.
5	IE(M,4)	+	id of the global node that serves as the 4 th element node of the global element.
10	IE(M,9)	+	The material ID of this element.

<u>GN Card</u>		<u>Mesh node</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GN	Card group identifier Mesh node. One entry for each node in the mesh.
1	NP	+	id of global node.
2	X(NP,1)	±	The x coordinate of the node [L].
3	X(NP,2)	±	The y coordinate of the node [L].
4	X(NP,3)	±	The z coordinate of the node [L].

<u>EN Card</u>		<u>End card</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	EN	Card group identifier
C 3	IC3	D	End of input data marker

I.2. File 2: 2-D overland geometry file (.2dm)

<u>Value</u>	<u>Description</u>
WMS2DM	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>GE Card</u>		<u>Element information</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GE	Card group identifier.

C 3	IC3		Identification of element.
		3	A triangular element is being input.
		4	A quadrilateral element is being input.
1	M	+	id of global element.
2	IE1(M,1)	+	id of the global node that serves as the 1 st element node of the global element.
3	IE2(M,2)	+	id of the global node that serves as the 2 nd element node of the global element.
4	IE2(M,3)	+	id of the global node that serves as the 3 rd element node of the global element.
5	IE2(M,4)	+	id of the global node that serves as the 4 th element node of the global element. It is zero for a triangular element.
6	IE2(M,5)	+	id of the material type of the global element.

GN Card

Field Variable

C 1-2 IC1

C 3 IC3

1 N

2 X2(N,1)

3 X2(N,2)

4 X2(N,3)

Node information

Value Description

GN Card group identifier.

blank.

+

± The x-coordinate of the global node [L].

± The y-coordinate of the global node [L].

± The z-coordinate (bottom elevation) of the global node [L].

EN Card

Field Variable

C1-2 IC1

C 3 IC3

End of data control

Value Description

EN Card group identifier.

D End of input data.

I.3. File 3: 1-D river/stream geometry file (.1dm)

Value

WMS1DM

Description

File type identifier

T1-T3 Cards

Job title

Only one T1, T2, and T3 card can be used.

GE Card

Field Variable

C 1-2 IC1

C 3 IC3

1 M

2 IE1(M,1)

3 IE1(M,2)

4 IE1(M,3)

Element information

Value Description

GE Card group identifier.

2 Identification of element.

+

+

+

+

AppI-3

<u>GN Card</u>		<u>Node information</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GN	Card group identifier.
C 3	IC3		blank
1	N	+	id of Global node.
2	X1(N,1)	+	The x-coordinate of the global node [L].
3	X1(N,2)	+	The z-coordinate (bottom elevation) of the global node [L].

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

I.4. File 4: 3-D subsurface flow file (.3bc file)

<u>Value</u>	<u>Description</u>
WMS3BC	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>OP Card</u>		<u>Run option parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier
C 3	IC3	1	Specify the type of simulation;
1	KMOD		Index of subsurface simulation.
		0	No subsurface simulation.
		1	Only flow is simulated.
		2	Both flow and transport are simulated.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier
C 3	IC3	2	Solver options.
1	KSSF	0	Steady-state flow simulation,
		1	Transient flow simulation;
2	ILUMP	0	No mass lumping,
		1	Mass lumping,
3	IPNTSF		Matrix solver for flow simulations.
		1	The pointwise iterative matrix solver
		2	Preconditioned Conjugate Gradient Method (polynomial),
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
4	IQUAR		Index of using quadrature for numerical integration.
		11	Nodal quadrature for the integration of an element face and an element.
		12	Nodal quadrature for the integration of an element face, Gaussian quadrature for the integration of an element.
		21	Gaussian quadrature for the integration of an element face, Nodal quadrature for the integration of an element.

5	IMODEL	22	Gaussian quadrature for the integration of an element face and an element.
			Index of simulating subsurface flow.
		-10	The flow equation is not solved. Rather, the pressure (total) head, Darcy velocity (specific discharge), and moisture content are given through the input of initial conditions.
		Otherwise	The flow equation is solved by using the Gelarkin finite element method.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier
C 3	IC3	3	Weighting factor for flow simulations;
1	WF		Time derivative weighting factor for flow simulations.
		0.5	Crank-Nicolson central
		1.0	Backward difference
2	OMEF		Iteration parameter for solving nonlinear matrix equations.
		0.0-1.0	Under relaxation,
		1.0	Exact relaxation,
		1.0-2.0	Over relaxation.
3	OMIF		Iteration parameter for solving linearized matrix equation pointwise.
		0.0-1.0	Under relaxation,
		1.0	Exact relaxation,
		1.0-2.0	Over relaxation.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier
C 3	IC3	4	Index for analytical soil characteristic function KSP;
1	KSP	0	KSP = 0 is an index for providing an analytical soil characteristic function .The default value is 1.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier
C 3	IC3	5	Parameters for Preconditioned Conjugate Gradient method;
1	IEIGEN	0	GG will not be read.
		1	GG will be read.
2	GG	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

<u>IP Card</u>		<u>Iteration Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IP	Card group identifier
C 3	IC3	1	Iteration parameters for solving flow equations
1	NITERF	+	Number of iterations allowed for solving the non-linear flow equation.
2	NCYLF	+	Number of cycles permitted for iterating rainfall seepage boundary condition or the boundary condition on the interface between 2-D overland and 3-D subsurface regimes per time step.
3	NPITERF	+	Number of iterations permitted for solving the linearized flow equations , i.e., this value is used in matrix solver.
4	TOLAF	+	The convergent criteria for the implementation of iteration scheme in the steady-state flow simulation [L].

5	TOLBF	+	The convergent criteria for the implementation of iteration scheme in the transient-state flow simulation [L].
6	V_CUT	+	Cut-off of velocity [L/T]. If the computed velocity is smaller than this value , it is set to zero.

TC Card

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	TMAX
2	DELT
3	DELTT

Iteration Parameters

<u>Value</u>	<u>Description</u>
TC	Card group identifier
1	Total simulation time and fixed time step size.
+	Maximum simulation time [T].
+	Initial time step size for flow [T].
+	Time step size for transport [T].

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	IDTXY

<u>Value</u>	<u>Description</u>
TC	Card group identifier.
2	Computational time step.
+	Index of xy series for variable time step.

OC Card

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	IBUG
2	ICHNG
3	JOPT
4	KPRT
	NPRINT
(new line)	

Output control parameters

<u>Value</u>	<u>Description</u>
OC	Card group identifier
1	Print control parameters.
0	Do not print the diagnostic output,
1	Do print the diagnostic output,
0	Do not print cyclic change of rainfall/seepage nodes or of ground surface nodes.
1	Print cyclic change of rainfall/seepage nodes or of ground surface nodes.
0	Print at specified interval,
1	Print at specified set of time values,
+	Specify the interval if JOPT = 0,
+	Specify total number of the specified times, if JOPT=1,
+	After OC1 card, specify the times, if JOPT = 1. One data entry per line.

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	NSELT
2	KPRO(i)

<u>Value</u>	<u>Description</u>
OC	Card group identifier
2	Print options.
+	Total options to be selected.
	Print options.
1	Print total head.
2	Print pressure head.
3	Print Darcy velocity (specific discharge).
4	Print nodal moisture content.
5	Print concentration.

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	IFILE

<u>Value</u>	<u>Description</u>
OC	Card group identifier
3	Output control for post-process.
0	Save as ASCII test format.

		1	Save as binary format.
2	KOPT	0	Save at specified interval.
		1	Save at specified set of times.
3	KDSK	+	Save every specified interval, if KOPT=0.
	KPOST	+	Save at specified set of times, if KOPT=1.
(new line)		+	After OC3 card, specify the times, if KOPT = 1. One data entry per line, up to KPOST times.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OC	Card group identifier
C 3	IC3	4	Solution file output options.
1	KSELT	+	Total options to be selected.
2	KSAVE(i)		Save options.
		0	Save nothing.
		1	Save pressure head.
		3	Save nodal moisture content.
		4	Save velocity.
		5	Save concentration.

<u>MP Card</u>		<u>Material property parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier
C 3	IC3	1	Index of hydraulic conductivity or permeability.
1	KCP	0	Hydraulic conductivity.
		1	Permeability.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier
C 3	IC3	2	Hydraulic conductivity or permeability tensor.
1	I	+	Material ID.
2	PROPF(1,I)	+	Saturated xx hydraulic conductivity, Kxx [L/T], or saturated permeability [L ²] of the medium I.
3	PROPF(2,I)	+	Saturated yy hydraulic conductivity, Kyy [L/T], or saturated permeability [L ²] of the medium I.
4	PROPF(3,I)	+	Saturated zz hydraulic conductivity Kzz [L/T], or saturated permeability [L ²] of the medium I.
5	PROPF(4,I)	+	Saturated xy hydraulic conductivity Kxy [L/T], or saturated permeability [L ²] of the medium I.
6	PROPF(5,I)	+	Saturated xz hydraulic conductivity Kxz [L/T], or saturated permeability [L ²] of the medium I.
7	PROPF(6,I)	+	Saturated yz hydraulic conductivity Kyz [L/T], or saturated permeability [L ²] of the medium I.
8	PROPF(9,I)	+	The effective porosity of the medium I, n _e [L ³ /L ³].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier
C 3	IC3	3	Density and viscosity of fresh water.
1	ITUNIT		Index of time unit.

		1	The time unit for simulation is second.
		2	The time unit for simulation is minute.
		3	The time unit for simulation is hour.
2	ILUNIT		Index of length unit.
		1	The length unit for simulation is meter.
		2	The length unit for simulation is foot.
		3	The length unit for simulation is kilometer.
		4	The length unit for simulation is mile.
3	RHO	+	Density of fresh water [M/L ³].
4	VISC	+	Dynamic viscosity of water [M/L/T].

SP Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	i
2	IHM(i)
3	IHC(i)
4	IHW(i)
5	HCON(i)
6	HMIN(i)

Soil property parameters for unsaturated zone

Value	Description
SP	Card group identifier
1	Soil property functions
+	Material type ID.
+	Index of moisture content vs. pressure head xy series.
+	Index of relative hydraulic conductivity vs. pressure head xy series.
+	Index of water capacity vs. pressure head xy series.
+	The ponding depth associated with the i th material.
±	The minimum pressure head associated with the i th material.

Note: This information is a MUST to perform subsurface simulations.

PS Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	NPWF(I)
2	IWTYPF(I)

Point source/sink parameters

Value	Description
PS	Card group identifier
1	Point source/sink flow rate for both flow and transport simulation.
+	Node number of the I th point source/sink.
+	Index of the flow rate xy series.

DB Card

Field	Variable
C 1-2	IC1
C3	IC3
1	NPDBF(I)
2	IDTYPF(I)
3	IDHB(I)

Dirichlet boundary parameters

Value	Description
DB	Card group identifier
1	Dirichlet boundary conditions, prescribed total head for flow simulation.
+	Global node number of the I th Dirichlet boundary,
+	Index of the head xy series.
	Index of the profile type for the j th Dirichlet boundary node.
0	This profile is a time-dependent pressure head profile.
1	This profile is a time-dependent total head profile.

CB Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	M
2	IDCF(I)
3	ICTYPF(I)

Cauchy boundary parameters

Value	Description
CB	Card group identifier
1	Cauchy boundary conditions, prescribed flow flux rate for flow simulation.
+	Element number of the Cauchy boundary.
+	Element face ID of this boundary side.
+	Index of the flux rate xy series.

NB Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	M
2	IDNF(I)
3	INTYPF(I)

Neumann boundary parameters

Value	Description
NB	Card group identifier
1	Neumann boundary conditions, prescribed flow flux rate (due to pressure head difference) for flow simulation.
+	Element number of the Neumann boundary.
+	Element face ID of this boundary side.
+	Index of the flux rate xy series.

RS Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	M
2	IDRF(I)
3	IVTYPF(I)

Variable boundary parameters

Value	Description
RS	Card group identifier
1	Variable boundary condition, rainfall/evaporation/seepage flux rate for flow simulation.
+	Element number of the rainfall/seepage boundary.
+	Element face ID of this boundary side.
+	Index number of rainfall/evaporation time series for the element face.

IC Card

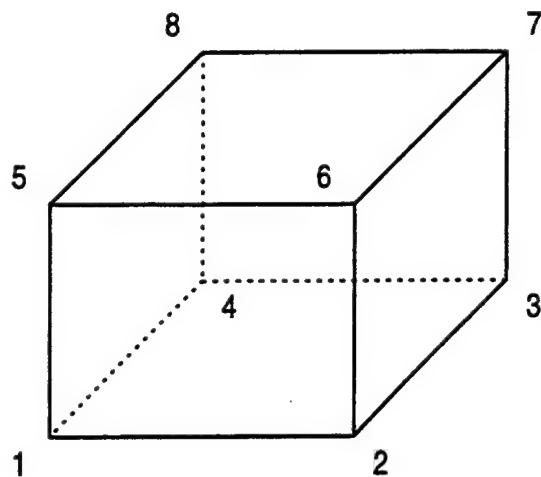
Field	Variable
C 1-2	IC1
C 3	IC3
1	ISTART

Initial condition data parameters

Value	Description
IC	Card group identifier
S	Initial condition start type.
0	Cold start.
1	Hot start.

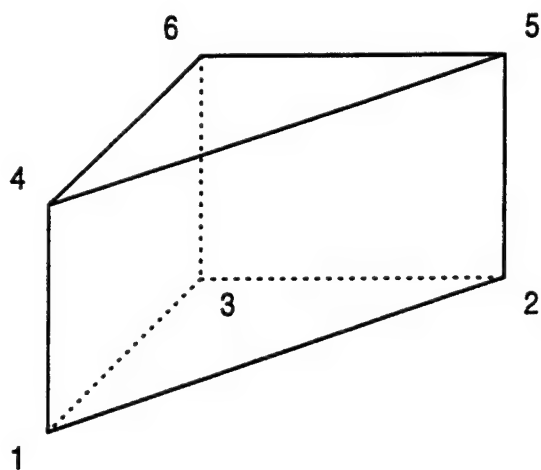
Field	Variable
C 1-2	IC1
C 3	IC3
1	HSTIME

Value	Description
IC	Card group identifier
T	Initial condition hot start time.
+	Time corresponding for the hot start.



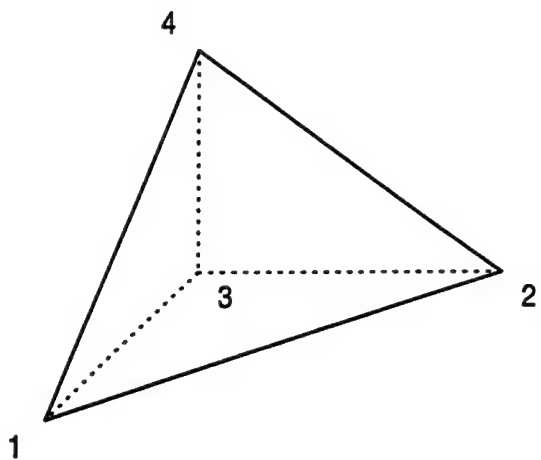
Hexahedral Element:

<u>Face</u>	<u>Nodes</u>
1	1-4-3-2
2	5-6-7-8
3	1-2-6-5
4	2-3-7-6
5	3-4-8-7
6	4-1-5-8



Triangular Prism Element:

<u>Face</u>	<u>Nodes</u>
1	1-3-2
2	4-5-6
3	1-2-5-4
4	2-3-6-5
5	3-1-4-6



Tetrahedral Element:

<u>Face</u>	<u>Nodes</u>
1	2-3-4
2	1-4-3
3	1-2-4
4	1-3-2

Figure I.1 Specification of 3-D element sides.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier
C 3	IC3	H	Constant or variable initial total head.
1	IHEAD	0	Constant total head.
		1	Spatially variable total head (if IDHEAD = 1) or pressure head (if IDHEAD = 0).
2	IDHEAD	0	Initial pressure head is to input.
		1	Initial total head is to input.
2	HCONST	±	If IHEAD=0, the constant head value. Otherwise, omit.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier
C3	IC3	U	Constant or variable initial velocity.
1	IVEL	0	Constant velocity.
		1	Spatially variable velocity.
2	UCONST	±	If IVEL=0, the x-velocity. Otherwise, omit.
3	VCONST	±	If IVEL=0, the y-velocity. Otherwise, omit.
4	WCONST	±	If IVEL=0, the z-velocity. Otherwise, omit.

Note: This card is a MUST when IMODEL = -10 (i.e., the flow is not to be computed).

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier
C3	IC3	M	Constant or variable initial moisture content.
1	IMOIS	0	Constant moisture content.
		1	Spatially variable moisture content.
2	THCNST	±	If IMOIS=0, the moisture content value. Otherwise, omit.

Note: This card is a MUST only when IMODEL = -10 (i.e., the flow is not to be computed).

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier
C 3	IC3	F	Initial condition file format.
1	ICFILE	0	The initial condition files are in text format.
		1	The initial condition files are in binary format.
2	IVFILE	0	The initial flow files are in text format.
		1	The initial flow files are in binary format.
3	IFFU	0	Flow files contain a steady-state solution.
		1	Flow files contain a transient solution.

<u>XY Card</u>		<u>X-Y Series Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	XY	Card group identifier
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series,
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTAX	0	Dummy values.
4	DELTAY	0	Dummy values.

5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y		\pm, \pm	After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier
C 3	IC3	D	End of input data

I.5. File 5: 2-D overland flow file (.2bc file)

<u>Value</u>	<u>Description</u>
WMS2BC	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>OP Card</u>		<u>Run option parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	1	Simulation selection.
1	KMOD		Index of river/stream simulation.
		0	No river/stream simulation.
		1	Only flow is simulated.
		2	Both flow and transport are simulated.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	2	Solver specification.
1	ILUMP		Index of using mass lumping.
		0	No mass lumping.
		1	Mass lumping.
2	IPNTS		Index of using linear matrix solver for flow simulations.
		1	The pointwise iterative matrix solver.
		2	Preconditioned Conjugate Gradient Method (polynomial).
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3	IQUAR		Index of using quadrature for numerical integration.
		1	Nodal quadrature for line element integration.
		2	Gaussian quadrature for line element integration.
4	IDIFF		Index of taking into account the eddy viscosity terms.
		1	Yes.
		0	No, the eddy viscosity terms are neglected.
5	IALLOW		Index of allowing the simulation to continue when there is no convergence reached for the non-linear iteration.
		1	Yes.

6	IMODEL	0	No.
			Index of simulating overland flow.
		3	Using MOC to solve the dynamic model only.
		2	Using the diffusion model only.
		1	Using the kinematic model only.
		-10	Specifying water depth and flow velocity with the initial condition. The flow equation is not solved.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	3	Weighting factor for simulations.
1	W		Time derivative weighting factor for flow simulation.
		0.5	Crank-Nicolson central.
		1.0	Backward difference.
2	OME		Relaxation parameter for solving nonlinear matrix equations.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.
3	OMI		Relaxation parameter for solving linearized matrix equation.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGEN	0	GG will not be read.
		1	GG will be read.
2	GG	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	5	Method of characteristics.
1	ISK		Index of choosing the directions of characteristics.
		-1	Using the velocity direction as the direction of characteristics.
		0	Solve the diagonalization equations for the directions.
		1	Specify directions by users.
2	ANGLE1	+	User specified angle (in degree) for the direction of the first characteristic. (COS(ANGLE1), SIN(ANGLE1)) is the direction.
3	ANGLE2	+	User specified angle (in degree) for the second and third characteristics. (COS(ANGLE2), SIN(ANGLE2)) is the direction.

<u>IP Card</u>		<u>Iteration Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IP	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NNITER	+	Allowed number for the non-linear iteration in the flow simulation.

2	NPITER	+	Allowed number for the linearized iteration in the flow simulation.
3	TOLBH	+	Allowed relative error for water depth.
4	TOLBV	+	Allowed relative error for velocity components.
5	V_CUT	+	Cut-off of velocity [L/T]. If the computed velocity is smaller than this value, it is set to zero.
6	FMSR	+	Multiplication factor to set the allowed mean square root errors, BHMSR for water depth and BVMSR for velocity, where BHMSR = TOLBH*FMSR; BVMSR = TOLBV*FMSR.

PT Card

Field Variable

C 1-2 IC1
C 3 IC3
1 NXW

2 IDETQ

Time marching parameters

Value Description

PT Card group identifier.
1 Total simulation time.
+ Subelement number in one direction that is used in the "in-element" particle tracking. The total subelement number included in one global element is NXW*NXW.
Index of particle tracking approach.
1 Using the average-velocity approach.
2 Using the constant-velocity approach.

TC Card

Field Variable

C 1-2 IC1
C 3 IC3
1 TMAX
2 DELT

Iteration Parameters

Value Description

TC Card group identifier.
1 Total simulation time.
+ Maximum simulation time [T].
+ Initial time step size [T].

Field Variable

C 1-2 IC1
C 3 IC3
1 IDTXY

Value Description

TC Card group identifier.
2 Computational time step.
+ Index of xy series for variable time step.

OC Card

Field Variable

C 1-2 IC1
C 3 IC3
1 IBUG
2 JOPT
3 KPRT
NPRINT

Output control parameters

Value Description

OC Card group identifier.
1 Print control parameters.
0 Do not print the diagnostic output.
1 Do print the diagnostic output.
0 Print at specified intervals.
1 Print at specified set of time values.
+ Specify the interval if JOPT = 0.
+ Specify total number of the specified times, if JOPT=1.

Note: NPRINT new lines after OC1 card are needed if JOPT = 1.
(the first new line)

1 TPRT(1) + The 1st specified time moment at which the associated simulation results are to be printed.

(the second new line)

1 TPRT(2) + The 2nd specified time moment at which the associated simulation results are to be printed.

(the NPRINT new line)

1 TPRT(NPRINT) + The NPRINTth specified time moment at which the associated simulation results are to be printed.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier
C 3	IC3	2	Print options.
1	NSELT	+	Total options to be selected.
2	KPRO(i)		Print options.
		1	Print water depth.
		2	Print velocity.
		3	Print concentration.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	3	Output control for post-process.
1	IFILE	0	Save as ascii format.
		1	Save as binary format.
2	KOPT	0	Save at specified interval.
		1	Save at specified set of times.
3	KDSK	+	Save every specified interval, if KOPT=0.
	NPOST	+	Save at specified set of times, if KOPT=1.

Note: NPOST new lines after OC3 card are needed if KOPT = 1.

(the first new line)

1 TSV(1) + The 1st specified time moment at which the associated simulation results are to be saved.

(the second new line)

1 TSV(2) + The 2nd specified time moment at which the associated simulation results are to be saved.

(the NPOST new line)

1 TSV(NPOST) + The NPOSTth specified time moment at which the associated simulation results are to be saved.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	4	Solution file output options.
1	KSELT	+	Total options to be selected.
2	KSAVE(i)		Save options.
		1	Save water depth.
		2	Save flux.
		3	Save infiltration rate.

GC Card

Cross section parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	1	Generate cross section to calculate discharge.
1	NGCL	+	Total number of cross sections.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	2	Cross section information.
1	id	+	Index number of cross section.
2	NPL	+	Number of nodal points in the x-section.
(new line)		+	Node points.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	3	Save and print hydrograph.
1	LOPT	0	Save and print at specified interval.
		1	Save and print at specified set of times.
2	LDSK	0	Save and print at specified interval.
		+	Save and print every specified interval, if LOPT=0.
	LPOST	+	Save and print at specified set of times, if LOPT=1.

Note: LPOST new lines after GC3 card are needed if LOPT = 1.

(the first new line)

1	TSA(1)	+	The 1 st specified time moment at which the associated hydrographs are to be saved.
---	--------	---	--

(the second new line)

1	TSA(2)	+	The 2 nd specified time moment at which the associated hydrographs are to be saved.
---	--------	---	--

(the NPOST new line)

1	TSA(LPOST)	+	The LPOST th specified time moment at which the associated hydrographs are to be saved.
---	------------	---	--

(new line)		+	After GC3 card, specify the times, if LOPT = 1. One data entry per line.
------------	--	---	--

MP Card

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	1	Material property.
1	i	+	id of material type.
2	PROP(1,i)	+	Manning's roughness associated with the material type.
3	PROP(2,i)	+	xx-eddy viscosity associated with the material type $[L^2/T]$.
4	PROP(3,i)	+	yy-eddy viscosity associated with the material type $[L^2/T]$.
5	PROP(4,i)	+	xy-eddy viscosity associated with the material type $[L^2/T]$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	2	Density of water and acceleration of gravity.
1	ITUNIT		Index of time unit.

2	ILUNIT	1	The time unit for simulation is second.
		2	The time unit for simulation is minute.
		3	The time unit for simulation is hour.
3	RHO		Index of length unit.
		1	The length unit for simulation is meter.
		2	The length unit for simulation is foot.
		3	The length unit for simulation is kilometer.
		4	The length unit for simulation is mile.
		+	Density of water [M/L ³].

RF Card

Field Variable

C 1-2 IC1
C 3 IC3
1 i
2 IRTYP(i)

Rainfall parameters

Value Description

RF Card group identifier.
1 Rainfall data for the simulation.
+ id of global element.
+ id of xy series to describe the time-dependent rainfall rate for the element.

SS Card

Field Variable

C 1-2 IC1
C 3 IC3
1 i
2 ISR(i)

Source/sink parameters

Value Description

SS Card group identifier.
1 Source/sink data for the simulation.
+ id of global node.
+ id of xy series to describe the time-dependent source/sink rate for the node.

OB Card

Field Variable

C 1-2 IC1
C 3 IC3
1 NPDB(j)
2 IDTYP(j)

3 IDHB(j)

Open boundary parameters

Value Description

OB Card group identifier.
1 Dirichlet boundary nodes for the simulation.
+ id of global node corresponding to the jth Dirichlet boundary node.
+ id of xy series to describe the time-dependent water stage or water depth profile associated with the Dirichlet boundary node.
Index of the profile type for the jth Dirichlet boundary node.
0 This profile is a time-dependent water depth profile.
1 This profile is a time-dependent water stage profile.

Field Variable

C 1-2 IC1
C 3 IC3
1 NSCB(j,1)

2 NSCB(j,2)

3 NSCB(j,3)

Value Description

OB Card group identifier.
2 Flux-type boundary sides for the simulation.
+ id of global node corresponding to the 1st node of the jth flux-type boundary side.
+ id of global node corresponding to the 2nd node of the jth flux-type boundary side.
id of the type for the jth flux-type boundary side.
1 This is a upstream boundary side with the time-dependent incoming normal flux specified.
2 This is a downstream boundary side with the water depth-dependent outgoing normal flux specified.

		3	This is either a river/stream-related or a river/stream junction-related boundary side with the water depth-dependent outgoing normal flux (when overland water and river/stream water are separated) or stage difference-dependent normal flux (when overland water and river/stream water are connected) specified.
4	ICTYP(j,1)	+	id of xy series to describe the time-dependent normal flux profile associated with the open boundary side when NSCB(j,3) = 1.
5	ICTYP(j,2)	+	id of xy series to describe the water depth-dependent normal flux profile associated with the open boundary side when NSCB(j,3) = 2, or 3 (for the case that river/stream and overland waters are separated).
6	ICTYP(j,3)	+	id of xy series to describe the water stage difference-dependent normal flux profile associated with the open boundary side when NSCB(j,3) = 3 (for the case that river/stream and overland waters are connected).

IC Card

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	H	Water depth or water stage.
1	IHEAD	0	Constant water depth or water stage.
		1	Variable water depth or water stage.
2	IDHEAD	0	Initial water depth is input.
		1	Initial water stage is input.
3	HCONST	+	Value of the constant water depth or water stage for IHEAD = 0 [L].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	U	Velocity.
1	IV	0	Constant velocity.
		1	Variable velocity.
2	UCONST	+	Value of the constant velocity [L/T].
3	VCONST	+	Value of the constant velocity [L/T].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	S	Initial condition start type.
1	ISTART	0	Cold start, water depth/water stage and velocity.
		1	Hot start, water stage and velocity.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	T	Initial condition start time.
1	HSTIME	+	Time corresponding for the hot start.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	F	Initial condition start type.
1	ICFILE	0	Text format.
		1	Binary format.

<u>XY Card</u>		<u>X-Y Series Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTA X	0	Dummy values.
4	DELTA Y	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

L.6. File 6: 1-D river/stream flow file (.1bc file)

<u>Value</u>	<u>Description</u>
WMS1BC	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>OP Card</u>		<u>Run option parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	1	Simulation selection.
1	KMOD		Index of river/stream simulation.
		0	No river/stream simulation.
		1	Only flow is simulated.
		2	Both flow and transport are simulated.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	2	Solver specification.
1	ILUMP		Index of using mass lumping.
		0	No mass lumping.
		1	Mass lumping.
2	IPNTS		Index of using linear matrix solver for flow simulations.
		1	The pointwise iterative matrix solver.
		2	Preconditioned Conjugate Gradient Method (polynomial),
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).

3	IQUAR	1	Index of using quadrature for numerical integration. Nodal quadrature for line element integration.
		2	Gaussian quadrature for line element integration.
4	IDIFF		Index of taking into account the eddy viscosity terms.
		1	Yes.
		0	No, the eddy viscosity terms are neglected.
5	IALLOW		Index of allowing the simulation to continue when there is no convergence reached for the non-linear iteration.
		1	Yes.
		0	No.
6	IMODEL		Index of simulating overland flow.
		3	Using MOC to solve the dynamic model only.
		2	Using the diffusion model only.
		1	Using the kinematic model only.
		-10	Specifying water depth and velocity as the initial conditions. The flow equation is not solved.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	3	Weighting factor for simulations.
1	W		Time derivative weighting factor for flow simulation.
		0.5	Crank-Nicolson central.
		1.0	Backward difference.
2	OME		Relaxation parameter for solving nonlinear matrix equations.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.
3	OMI		Relaxation parameter for solving linearized matrix equation.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGEN	0	GGT will not be read.
		1	GGT will be read.
2	GG	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

<u>IP Card</u>		<u>Iteration Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IP	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NNITER	+	Allowed number for the non-linear iteration in the flow simulation.
2	NPITER	+	Allowed number for the linearized iteration in the flow simulation.
3	TOLBH	+	Allowed relative error for water depth.
4	TOLBV	+	Allowed relative error for velocity components.

5	V_CUT	+	Cut-off of velocity [L/T]. If the computed velocity is smaller than this value, it is set to zero.
6	FMSR	+	Multiplication factor to set the allowed mean square root errors, BHMSR for water depth and BVMSR for velocity, where BHMSR = TOLBH*FMSR; BVMSR = TOLBV*FMSR.

PT Card

Particle tracking parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	PT	Card group identifier.
C 3	IC3	1	Particle tracking controlling parameters.
1	NXW	+	Subelement number used in the X-direction in the "in-element" particle tracking.
2	IDETQ		Index of particle tracking approach.
		1	Using the average-velocity approach.
		2	Using the constant-velocity approach.

TC Card

Iteration Parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	TC	Card group identifier.
C 3	IC3	1	Total simulation time.
1	TMAX	+	Maximum simulation time [T].
2	DELT	+	Initial time step size [T].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	TC	Card group identifier.
C 3	IC3	2	Computational time step.
1	IDTXY	+	Index of xy series for variable time step.

OC Card

Output control parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	1	Print control parameters.
1	IBUG	0	Do not print the diagnostic output.
		1	Do print the diagnostic output.
2	JOPT	0	Print at specified interval.
		1	Print at specified set of time values.
3	KPRT	+	Specify the interval if JOPT = 0.
	NPRINT	+	Specify total number of the specified times, if JOPT=1.

Note: NPRINT new lines after OC1 card are needed if JOPT = 1.

(the first new line)

1	TPRT(1)	+	The 1 st specified time moment at which the associated simulation results are to be printed.
---	---------	---	---

(the second new line)

1	TPRT(2)	+	The 2 nd specified time moment at which the associated simulation results are to be printed.
---	---------	---	---

(the NPRINT new line)

1 TPRT(NPRINT) + The NPRINTth specified time moment at which the associated simulation results are to be printed.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OC	Card group identifier
C 3	IC3	2	Print options.
1	NSELT	+	Total options to be selected.
2	KPR0(i)		Print options.
		1	Print water depth.
		2	Print velocity/discharge.
		3	Print concentration.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	3	Output control for post-process.
1	IFILE	0	Save as ascii format.
		1	Save as binary format.
2	KOPT	0	Save at specified interval.
		1	Save at specified set of times.
3	KDSK	+	Save every specified interval, if KOPT=0.
	NPOST	+	Save at specified set of times, if KOPT=1.

Note: NPOST new lines after OC3 card are needed if KOPT = 1.
(the first new line)

1 TSV(1) + The 1st specified time moment at which the associated simulation results are to be saved.

(the second new line)

1 TSV(2) + The 2nd specified time moment at which the associated simulation results are to be saved.

(the NPOST new line)

1 TSV(NPOST) + The NPOSTth specified time moment at which the associated simulation results are to be saved.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	4	Solution file output options.
1	KSELT	+	Total options to be selected.
2	KSAVE(i)		Save options.
		1	Save water depth.
		2	Save flux.
		3	Save infiltration rate.

GC Card

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	1	Generate cross section to calculate discharge.
1	NGCL	+	Total number of cross sections.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	2	Cross section information.
1	id	+	Index number of cross section.
2	NPL	+	Number of nodal points in the x-section.
(new line)		+	Node points.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	3	Save and print hydrograph.
1	LOPT	0	Save and print at specified interval.
		1	Save and print at specified set of times.
2	LDSK	0	Save and print at specified interval.
		+	Save and print every specified interval, if LOPT=0.
3	LPOST	+	Save and print at specified set of times, if LOPT=1.

Note: LPOST new lines after GC3 card are needed if LOPT = 1.

(the first new line)

1	TSA(1)	+	The 1 st specified time moment at which the associated hydrographs are to be saved.
---	--------	---	--

(the second new line)

1	TSA(2)	+	The 2 nd specified time moment at which the associated hydrographs are to be saved.
---	--------	---	--

(the NPOST new line)

1	TSA(LPOST)	+	The LPOST th specified time moment at which the associated hydrographs are to be saved.
---	------------	---	--

(new line) + After GC3 card, specify the times, if LOPT = 1. One data entry per line.

MP Card

Material property parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	1	Material property.
1	i	+	id of material type.
2	PROP(1,i)	+	Manning's roughness associated with the material type.
3	PROP(2,i)	+	x-eddy viscosity associated with the material type [L^2/T].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	2	Density of water and acceleration of gravity.
1	ITUNIT		Index of time unit.
		1	The time unit for simulation is second.
		2	The time unit for simulation is minute.
		3	The time unit for simulation is hour.
2	ILUNIT		Index of length unit.
		1	The length unit for simulation is meter.
		2	The length unit for simulation is foot.
		3	The length unit for simulation is kilometer.

3	RHO	4	The length unit for simulation is mile.
		+	Density of water [M/L ³].

RF Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	i
2	IRTYP(i)

Rainfall parameters

Value	Description
RF	Card group identifier.
1	Rainfall data for the simulation.
+	id of global element.
+	id of xy series to describe the time-dependent rainfall rate for the element.

SS Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	i
2	ISR(i)

Source/sink parameters

Value	Description
SS	Card group identifier.
1	Source/sink data for the simulation.
+	id of global node.
+	id of xy series to describe the time-dependent source/sink rate for the node.

OB Card

Field	Variable
C 1-2	IC1
C3	IC3
1	NPDB(j,1)
2	NPDB(j,2)

Open boundary parameters

Value	Description
OB	Card group identifier.
1	Open boundary for the simulation.
+	id of global node corresponding to the j th open boundary node.
	id of the type for the open boundary node.
1	This is a boundary node with the time-dependent water stage specified.
2	This is a upstream boundary node with the time-dependent incoming normal flux specified.
3	This is a downstream boundary node with the water depth-dependent outgoing normal flux specified.
+	id of xy series to describe the time-dependent water stage or water depth profile associated with the open boundary node when NPDB(j,2) = 1.
+	id of xy series to describe the time-dependent normal flux profile associated with the open boundary node when NPDB(j,2) = 2.
+	id of xy series to describe the water depth-dependent normal flux profile associated with the open boundary node when NPDB(j,2) = 3.
	Index of the profile type for IDTYP(j,2) when NPDB(j,2) = 2.
0	This profile is a time-dependent water depth profile.
1	This profile is a time-dependent water stage profile.

CS Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	j
2	ICHN(j,1)
3	ICHN(j,2)
4	ICHN(j,3)

River/stream cross-sectional parameters

Value	Description
CS	Card group identifier.
1	Profile types for river/stream cross-sectional geometry.
+	id of river/stream node.
+	id of xy series to describe the water depth-dependent cross-sectional area profile for the river/stream node.
+	id of xy series to describe the water depth-dependent wetted perimeter profile for the river/stream node.
+	id of xy series to describe the water depth-dependent top river/stream width

profile for the river/stream node.

Note: The top river/stream width value at zero water depth must be GREATER than zero when describing the profile associated with it.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	CS	Card group identifier.
C 3	IC3	2	Entire river/stream width .
1	j	+	id of river/stream node.
2	CHNW(j)	+	The entire river/stream width through which rainfall can contribute to river/stream at the river/stream node. [L]

<u>RH Card</u>		<u>River/stream reach parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RH	Card group identifier.
C 3	IC3	1	River/stream nodes included in each river/stream reach.
1	j	+	id of river/stream reach.
2	nn	+	Number of nodes included in the river/stream reach.

Note: A river/stream reach must include at least four river/stream nodes.

Note: One new line after RH1 card is needed.

(new line, including nn data)

NPINRH(1..nn,j) +Node numbers of river/stream nodes that are included in the river/stream reach. These nodes must be given in order from the upstream to the downstream.

<u>JT Card</u>		<u>River/stream junctions</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	JT	Card group identifier.
C 3	IC3	1	parameters of junction geometry.
1	j	+	id of river/stream junction.

Note: A river/stream dead end is treated as a river/stream junction.

2	NPJT(j)	+	id of overland global node that is associated with the j th junction.
3	IVJT(j)	+	id of xy series to describe the volume-water depth relationat the river/stream junction.
4	IDJCNT(j)	1	This junction is to simulate a big lake and the water stage at junction's outlets are considered to be the same as the junction's.
		0	Otherwise.
5	AJT(j)	+	Horizontal area of the junction, through which both rainfall and infiltration can contribute to the change of water depth of the junction [L ²].
6	Z0JT(j)	+	Bottom elevation of the junction [L].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	JT	Card group identifier.
C 3	IC3	2	river/stream reaches and nodes associated with river/stream junctions.
1	j	+	id of river/stream junction.

Note: A river/stream dead end is treated as a river/stream junction.

2 NJTRH(j) + Number of river/stream reaches that connect to one another through the river/stream junction.

Note: If this river/stream junction is simulating a pond without outlet, NJTRH(j) = 0.

(new line) IDJT(1,1..nn,j) id of river/stream global nodes which coincide with the junction and are the end nodes of the reaches connected to the junction. (nn = NJTRH(j))

(new line) IDJT(2,1..nn,j) id of river/stream global nodes which are the nodes next to the nodes specified in IDJT(1,1..nn,j). (nn = NJTRH(j))

Note: IDJT(1,i,j) must match IDJT(2,i,j) for the ith reach connected to the jth junction.

Field	Variable	Value	Description
C 1-2	IC1	JT	Card group identifier.
C 3	IC3	3	junction-related overland boundary sides.
1	j	+	id of river/stream junction.

Note: A river/stream dead end is treated as a river/stream junction.

2 NJT12(j) + Number of junction-related overland boundary segments.

Note: nn new lines after JT3 card are needed, where nn = NJT12(j).

(the first new line)

1 NSJT12(1,1) + The 2-D global node that corresponds to the 1st node of the 1st surrounding overland boundary segment of the river/stream junction.

2 NSJT12(2,1) + The 2-D global node that corresponds to the 2nd node of the 1st surrounding overland boundary segment of the river/stream junction.

(the nnth new line)

1 NSJT12(1,nn) + The 2-D global node that corresponds to the 1st node of the nnth surrounding overland boundary segment of the river/stream junction.

2 NSJT12(2,nn) + The 2-D global node that corresponds to the 2nd node of the nnth surrounding overland boundary segment of the river/stream junction.

<u>IC Card</u>		<u>Initial condition data parameters</u>	
Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	H	Water depth or water stage.
1	IHEAD	0	Constant water depth or water stage.
		1	Variable water depth or water stage.
2	IDHEAD	0	Initial water depth is input.
		1	Initial water stage is input.
3	HCONST	+	Value of the constant water depth or water stage for IHEAD = 0 [L].

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	U	Velocity.
1	IV	0	Constant velocity.
		1	Variable velocity.
2	UCONST	±	Value of the constant velocity [L/T].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	S	Initial condition start type.
1	ISTART	0	Cold start, water depth/water stage and velocity.
		1	Hot start, water depth/water stage and velocity.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	T	Initial condition start time.
1	HSTIME	+	Time corresponding for the hot start [T].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	F	Initial condition start type.
1	ICFILE	0	Text format.
		1	Binary format.

<u>XY Card</u>		<u>X-Y Series Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTAX	0	Dummy values.
4	DELTAY	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

I.7. File 7: 3-D subsurface transport file (.3tp file)

<u>Value</u>	<u>Description</u>
WMS3TP	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>OP Card</u>		<u>Run option parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier

C 3	IC3	2	Solver options.
1	ILUMPT	0	No mass lumping,
		1	Mass lumping,
2	IPNTST		Matrix solver for flow and transport simulations.
		1	The pointwise iterative matrix solver
		2	Preconditioned Conjugate Gradient Method (polynomial),
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3	IQUART		Index of using quadrature for numerical integration.
		11	Nodal quadrature for the integration of an element face and an element.
		12	Nodal quadrature for the integration of an element face, Gaussian quadrature for the integration of an element.
		21	Gaussian quadrature for the integration of an element face, Nodal quadrature for the integration of an element.
		22	Gaussian quadrature for the integration of an element face and an element.
4	IADAPT		Index of using adapted implicit-explicit scheme for the predictor step.
		0	No.
		1	Yes.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier
C 3	IC3	3	Weighting factor for flow and transport simulations;
1	WT		Time derivative weighting factor for flow and transport simulation,
		0.5	Crank-Nicolson central
		1.0	Backward difference
2	OMET		Iteration parameter for solving nonlinear matrix equations.
		0.0-1.0	Under relaxation,
		1.0	Exact relaxation,
		1.0-2.0	Over relaxation.
3	OMIT		Iteration parameter for solving linearized matrix equation pointwise.
		0.0-1.0	Under relaxation,
		1.0	Exact relaxation,
		1.0-2.0	Over relaxation.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier
C 3	IC3	5	Parameters for Preconditioned Conjugate Gradient method;
1	IEIGENT	0	GGT will not be read.
		1	GGT will be read.
2	GGT	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

IP Card

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IP	Card group identifier
C 3	IC3	2	Iteration parameters for solving transport equations
1	NITERT	+	Number of iterations allowed for solving the non-linear transport equation.
2	NPITERT	+	Number of iterations permitted for solving the linearized transport equations, i.e., this value is used in matrix solver.

3	TOLBT	+	The convergent criteria (allowed relative error) for the implementation of iteration scheme in the transient-state transport simulation.
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PT Card

Particle Tracking Parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	PT	Card group identifier
C 3	IC3	1	Particle tracking parameters
1	NXW	+	The number of grids for sub-element tracking in the x-direction.
2	IDETQ		Index of particle tracking velocity.
		1	Average velocity of starting and ending points is used.
		2	Single velocity of starting point is used.

MP Card

Material property parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	MP	Card group identifier
C 3	IC3	5	Dispersion/diffusion coefficients.
1	I	+	Material type ID.
2	PROPT(1,I)	+	Bulk density, ρ_b for medium I [M/L^3].
3	PROPT(2,I)	+	Longitudinal dispersion, a_L for medium I [L].
4	PROPT(3,I)	+	Transverse dispersion, a_T for medium I [L].
5	PROPT(4,I)	+	Molecular diffusion coefficient, a_M for medium I [L^2/T].
6	PROPT(5,I)	+	Tortuosity, τ for medium I [dimensionless].
7	PROPT(6,I)	+	The effective porosity of the medium I, n_e [L^3/L^3].

PS Card

Point source/sink parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	PS	Card group identifier
C 3	IC3	2	Point source/sink concentration for transport simulation.
1	ID	+	id of point source/sink.
2	NPWT(ID)	+	Node number of the I^{th} point source/sink,
3	NCHEM	+	Number of dissolved chemicals.

(NCHEM more lines are needed. Each line contains the following information.

1	i	+	id of dissolved chemical.
2	IWTYPT(ID,i)	+	Index of the source rate xy series.

DB Card

Dirichlet boundary parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DB	Card group identifier.
C 3	IC3	2	Dirichlet boundary conditions, prescribed concentration for transport simulation.
1	NP	+	id of Dirichlet boundary node.
2	NPDBT(NP)	+	id of global node corresponding to the Dirichlet boundary node.
3	NCHEM	+	Number of dissolved chemicals.

(NCHEM more lines are needed. Each line contains the following information.

1	i	+	id of dissolved chemical.
2	IDTYPT(NP,i)	+	id of xy series to described the time-dependent concentration profile

associated with the Dirichlet boundary node for the dissolved chemical.

<u>CB Card</u>		<u>Cauchy boundary parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	CB	Card group identifier
C 3	IC3	2	Cauchy boundary conditions, prescribed mass flux rate for transport simulation.
1	NS	+	id of Cauchy boundary side.
2	M	+	id of global element corresponding to the Cauchy boundary side.
3	IDCT(NS)	+	id of element face corresponding to the Cauchy boundary side (ranging from 1 to 6).
4	NCHEM	+	Number of dissolved chemicals.

(NCHEM more lines are needed. Each line contains the following information.

1	i	+	id of dissolved chemical.
2	ICTYPT(NS,i)	+	id of xy series to described the time-dependent concentration flux profile associated with the Cauchy boundary side for the dissolved chemical.

<u>NB Card</u>		<u>Neumann boundary parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	NB	Card group identifier
C 3	IC3	2	Neumann boundary conditions, prescribed dispersive mass flux rate for transport simulation.
1	NS	+	id of Neumann boundary side.
2	M	+	id of global element corresponding to the Neumann boundary side.
3	IDNT(NS)	+	id of element face corresponding to the Neumann boundary side (ranging from 1 to 6).
4	NCHEM	+	Number of dissolved chemicals.

(NCHEM more lines are needed. Each line contains the following information.

1	i	+	id of dissolved chemical.
2	INTYPT(NS,i)	+	id of xy series to described the time-dependent concentration flux profile associated with the Neumann boundary side for the dissolved chemical.

<u>RS Card</u>		<u>Variable boundary parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RS	Card group identifier
C 3	IC3	2	Variable boundary conditions, prescribed concentration for transport simulation.
1	NS	+	id of Variable boundary side.
2	M	+	id of global element corresponding to the Variable boundary side.
3	IDNT(NS)	+	id of element face corresponding to the Variable boundary side (ranging from 1 to 6).
4	NCHEM	+	Number of dissolved chemicals.

(NCHEM more lines are needed. Each line contains the following information.

1	i	+	id of dissolved chemical.
2	INTYPT(NS,i)	+	id of xy series to described the time-dependent concentration flux associated

with the Variable boundary side for the dissolved chemical.

IC Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	IDCONC

Initial condition data parameters

Value	Description
IC	Card group identifier
1	Constant or variable initial concentration.
0	Constant initial concentration.
1	Spatially variable initial concentration.

Field	Variable
C 1-2	IC1
C 3	IC3
1	j
2	CCONST(j)

Value	Description
IC	Card group identifier.
2	Initially constant conditions for dissolved chemicals.
+	id of the dissolved chemical being input.
+	Specified initial concentration for the dissolved chemical. [M/L ³].

Field	Variable
C 1-2	IC1
C 3	IC3
1	j
2	SITCON(j)

Value	Description
IC	Card group identifier.
3	Initially constant conditions for adsorbing sites.
+	id of the adsorbing site being input.
+	Specified initial concentration for the adsorbing site. [M/L ³].

Field	Variable
C 1-2	IC1
C 3	IC3
1	j
2	SORCON(j)

Value	Description
IC	Card group identifier.
4	Initially constant conditions for adsorbed chemicals.
+	id of the adsorbed chemical being input.
+	Specified initial concentration for the adsorbed chemical. [M/L ³].

Field	Variable
C 1-2	IC1
C 3	IC3
1	ICFILE

Value	Description
IC	Card group identifier
F	Initial condition file format.
0	The initial condition files are in text format.
1	The initial condition files are in binary format.

XY Card

Field	Variable
C 1-2	IC1
C 3	IC3
1	i
2	NPOINT(i)
3	DELTA X
4	DELTA Y
5	REPEAT
6	BEGCYC
7	TNAME

X-Y Series Parameters

Value	Description
XY	Card group identifier
1	Generation of any x-y series function.
+	Index number for x-y series,
+	The number of x-y values in the series.
0	Dummy values,
0	Dummy values,
0	Dummy values,
0	Dummy values,
+	A character string representing the name of the XY series.
±, ±	After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

EN Card

End of data control

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier
C 3	IC3	D	End of input data

I.8. File 8: 2-D overland transport file (.2tp file)

<u>Value</u>	<u>Description</u>
WMS2TP	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>OP Card</u>		<u>Run option parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	1	Simulation selection.
1	IDCHEM		Index of chemical transport simulation.
		0	Chemical transport is not simulated.
		1	Chemical transport is simulated.
2	IDSED		Index of sediment transport simulation.
		0	Sediment transport is not simulated.
		1	Sediment transport is simulated.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	2	Solver specification.
1	ILUMPT		Index of using mass lumping for transport simulations.
		0	No mass lumping.
		1	Mass lumping.
2	IPNTST		Index of using linear matrix solver for transport simulations.
		1	The pointwise iterative matrix solver.
		2	Preconditioned Conjugate Gradient Method (polynomial),
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3	IQUART		Index of using quadrature for numerical integration.
		1	Nodal quadrature for line element integration.
		2	Gaussian quadrature for line element integration.
4	IADAPT		Index of using adapted implicit-explicit scheme for the predictor step.
		0	No.
		1	Yes.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	3	Weighting factor for transport simulations.
1	WT		Time derivative weighting factor for transport simulation.
		0.5	Crank-Nicolson central.
		1.0	Backward difference.
2	OMET		Relaxation parameter for solving nonlinear matrix equations.

3	OMIT	0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.
			Relaxation parameter for solving linearized matrix equation.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGENT	0	GGT will not be read.
		1	GGT will be read.
2	GGT	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

<u>IP Card</u>		<u>Iteration Parameters</u>	
Field	Variable	Value	Description
C 1-2	IC1	IP	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NNITERT	+	Allowed number for the non-linear iteration.
2	NPITER	+	Allowed number for the linearized iteration.
3	TOLBC	+	Allowed relative error for getting convergent transport solutions for both dissolved and particulate chemicals.
4	TOLBS	+	Allowed relative error for getting convergent transport solutions for sediments.

<u>PT Card</u>		<u>Particle tracking parameters</u>	
Field	Variable	Value	Description
C 1-2	IC1	PT	Card group identifier.
C 3	IC3	1	Particle tracking controlling parameters.
1	NXWT	+	Subelement number in one direction that is used in the "in-element" particle tracking. The total subelement number included in one global element is NXWT*NXWT.
2	IDETQT		Index of particle tracking approach.
		1	Using the average-velocity approach.
		2	Using the constant-velocity approach.

<u>MP Card</u>		<u>Material property parameters</u>	
Field	Variable	Value	Description
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	1	Material property for transport.
1	i	+	id of material type.
2	PROPT(1,i)	+	Longitudinal dispersivity associated with the material type [L].
3	PROPT(2,i)	+	Lateral dispersivity associated with the material type [L].
4	PROPT(3,i)	+	Pure diffusion coefficient associated with the material type [L ² /T].

<u>SS card</u>	<u>Source/sink parameters</u>
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<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	1	Source/sink profile for dissolved chemicals.
1	NP	+	id of global node.
2	j	+	id of dissolved chemical.
3	ITSR(NP,j)	+	id of xy series to describe the time-dependent source/sink profile for the dissolved chemical at the global node.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	2	Source/sink profile for suspended sediment.
1	NP	+	id of global node.
2	j	+	id of suspended sediment size.
3	NCHEM	+	Number of dissolved chemicals.
4	ITSR(m)	+	id of xy series to describe the time-dependent source/sink profile for the suspended sediment size at the global node, where $m = NCHEM + j$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	3	Source/sink profile for particulate chemicals on suspended sediments.
1	NP	+	id of global node.
2	j	+	id of suspended sediment.
3	k	+	id of particulate chemical.
4	NCHEM	+	Number of dissolved chemicals.
5	NSSIZE	+	Number of sediment sizes.
6	ITSR(m)	+	id of xy series to describe the time-dependent source/sink profile for the particulate chemical on the suspended sediment size at the global node, where $m = NCHEM + NSSIZE + (j-1)*NCHEM + k$, $j \in [1, NSSIZE]$, and $k \in [1, NCHEM]$.

<u>DB Card</u>		<u>Dirichlet boundary parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DB	Card group identifier.
C3	IC3	1	Dirichlet boundary conditions for dissolved chemicals.
1	NP	+	id of Dirichlet boundary node.
2	NPDBT(NP)	+	id of global node corresponding to the Dirichlet boundary node.
3	i	+	id of dissolved Chemical.
4	IDTYPT(NP,i)	+	id of xy series to describe the time-dependent concentration profile associated with the Dirichlet boundary node for the dissolved chemical.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DB	Card group identifier.
C3	IC3	2	Dirichlet boundary conditions for suspended sediments.
1	NP	+	id of Dirichlet boundary node.
2	NPDBT(NP)	+	id of global node corresponding to the Dirichlet boundary node.
3	k	+	id of suspended sediment size.
4	NCHEM	+	Number of dissolved chemicals.
5	IDTYPT(NP,i)	+	id of xy series to describe the time-dependent concentration profile

associated with the Dirichlet boundary node for the suspended sediment, where $i = NCHEM + k$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DB	Card group identifier.
C 3	IC3	3	Dirichlet boundary conditions for particulate chemicals on suspended sediments.
1	NP	+	id of Dirichlet boundary node.
2	NPDBT(NP)	+	id of global node corresponding to the Dirichlet boundary node.
3	j	+	id of suspended sediment size.
4	k	+	id of particulate chemical.
5	NCHEM	+	Number of dissolved chemicals.
6	NSSIZE	+	Number of sediment sizes.
7	IDTYPT(NP,i)	+	id of xy series to describe the time-dependent concentration profile associated with the Dirichlet boundary node for the particulate chemical on the suspended sediment, where $i = NCHEM + NSSIZE + (j-1)*NCHEM + k$, $j \in [1, NSSIZE]$, and $k \in [1, NCHEM]$.

<u>FB Card</u>		<u>Flux-type boundary parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	FB	Card group identifier.
C 3	IC3	1	Flux-type boundary conditions for dissolved chemicals.
1	NS	+	id of flux-type boundary side.
2	NSCBT(NS,1)	+	id of global node corresponding to the 1 st node of the flux-type boundary side.
3	NSCBT(NS,2)	+	id of global node corresponding to the 2 nd node of the flux-type boundary side.
4	NSCBT(NS,3)		Index of boundary condition type for the flux-type boundary side.
		1	This is a Variable boundary side with the time-dependent concentration specified if the flow is incoming.
		2	This is a Cauchy boundary side with the time-dependent Cauchy flux specified.
		3	This is a Neumann boundary side with the time-dependent Neumann flux specified.
		4	This is a river/stream-related or a river/stream junction-related boundary side. The associated boundary conditions is a Variable boundary condition. However, the concentrations along with the inward flow are not prescribed. Rather they are the concentrations at the associated river/stream nodes or river/stream junction for the time being.
5	i	+	id of dissolved Chemical.
6	ICTYPT(NS,i)	+	id of xy series to describe the time-dependent profile associated with the flux-type boundary side for the dissolved chemical. It is (1) a concentration profile when NSCBT(j,2) = 1. (2) a Cauchy flux profile when NSCBT(j,2) = 2. (3) a Neumann flux profile when NSCBT(j,2) = 3.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	FB	Card group identifier.

C 3	IC3	2	Flux-type boundary conditions for suspended sediments.
1	NS	+	id of flux-type boundary side.
2	NSCBT(NS,1)	+	id of global node corresponding to the 1 st node of the flux-type boundary side.
3	NSCBT(NS,2)	+	id of global node corresponding to the 2 nd node of the flux-type boundary side.
4	NSCBT(NS,3)		Index of boundary condition type for the flux-type boundary side.
		1	This is a Variable boundary side with the time-dependent concentration specified if the flow is incoming.
		2	This is a Cauchy boundary side with the time-dependent Cauchy flux specified.
		3	This is a Neumann boundary side with the time-dependent Neumann flux specified.
		4	This is a river/stream-related or a river/stream junction-related boundary side. The associated boundary conditions is a Variable boundary condition. However, the concentrations along with the inward flow are not prescribed. Rather they are the concentrations at the associated river/stream nodes or river/stream junction for the time being.
5	k	+	id of suspended sediment size.
6	NCHEM	+	Number of dissolved chemicals.
7	ICTYPT(NS,i)	+	id of xy series to describe the time-dependent profile associated with the flux -type boundary side for the suspended sediment, <i>where i = NCHEM+k</i> . It is
			(1) a concentration profile when NSCBT(j,2) = 1.
			(2) a Cauchy flux profile when NSCBT(j,2) = 2.
			(3) a Neumann flux profile when NSCBT(j,2) = 3.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	FB	Card group identifier.
C3	IC3	3	Flux-type boundary conditions for particulate chemicals on suspended sediments.
1	NS	+	id of flux-type boundary side.
2	NSCBT(NS,1)	+	id of global node corresponding to the 1 st node of the flux-type boundary side.
3	NSCBT(NS,2)	+	id of global node corresponding to the 2 nd node of the flux-type boundary side.
4	NSCBT(NS,3)		Index of boundary condition type for the flux-type boundary side.
		1	This is a Variable boundary side with the time-dependent concentration specified if the flow is incoming.
		2	This is a Cauchy boundary side with the time-dependent Cauchy flux specified.
		3	This is a Neumann boundary side with the time-dependent Neumann flux specified.
		4	This is a river/stream-related or a river/stream junction-related boundary side. The associated boundary conditions is a Variable boundary condition. However, the concentrations along with the inward flow are not prescribed. Rather they are the concentrations at the associated river/stream nodes or river/stream junction for the time being.

5	j	+	id of suspended sediment size.
6	k	+	id of particulate chemical.
7	NCHEM	+	Number of dissolved chemicals.
8	NSSIZE	+	Number of sediment sizes.
9	ICTYPT(NS,i)	+	id of xy series to describe the time-dependent profile associated with the flux -type boundary side for the particulate chemical on the suspended sediment, where $i = NCHEM + NSSIZE + (j-1)*NCHEM + k$, $j \in [1, NSSIZE]$, and $k \in [1, NCHEM]$. It is (1) a concentration profile when NSCBT(j,2) = 1. (2) a Cauchy flux profile when NSCBT(j,2) = 2. (3) a Neumann flux profile when NSCBT(j,2) = 3.

RS card

Rainfall source parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RS	Card group identifier.
C 3	IC3	1	Rainfall source profile for dissolved chemicals.

1st line includes two records as follows.

1	M	+	id of 2-D element.
2	NCHEM	+	Number of dissolved chemicals.

2nd line includes NCHEM records as follows.

1	IRC(M,1)	+	id of xy series to describe the time-dependent concentration profile for the 1 st dissolved chemical in the rainfall that falls on the M th 2-D element.
2	IRC(M,2)	+	id of xy series to describe the time-dependent concentration profile for the 2 nd dissolved chemical in the rainfall that falls on the M th 2-D element.

Up to for the NCHEMth dissolved chemical on the Mth 2-D element.

IC card

Initial condition parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	1	Initial condition parameters.
1	IDCONC		id of initial concentrations.
		0	constant initial concentrations.
		1	variable initial concentrations.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	2	Initially constant conditions for dissolved chemicals.
1	j	+	id of the dissolved chemical being input.
2	CCONST(j)	+	Specified initial concentration for the dissolved chemical. [M/L ³]

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	3	Initially constant conditions for particulate chemicals on suspended sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the suspended sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	CCONST(k)	+	Specified initial concentration for the particulate chemical on suspended

sediment being input, where $k = i \cdot \text{NCHEM} + j$. $[\text{M/L}^3]$

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	4	Initially constant conditions for particulate chemicals on bed sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the bed sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	NSSIZE	+	Number of sediment sizes.
5	CCONST(k)	+	Specified initial concentration for the particulate chemical on the bed sediment being input, where $k = (i + \text{NSSIZE}) \cdot \text{NCHEM} + j$ $[\text{M/L}^3]$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	5	Initially constant conditions for suspended sediments.
1	i	+	id of the suspended sediment size being input.
2	SCONST(i)	+	Specified initial concentration for the suspended sediment of the i^{th} size. $[\text{M/L}^3]$

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	6	Initially constant conditions for bed sediments.
1	i	+	id of the bed sediment size being input.
2	NSSIZE	+	Number of sediment sizes.
3	SCONST(k)	+	Specified initial concentration for the bed sediment of the i^{th} size, where $k = \text{NSSIZE} + i$. $[\text{M/L}^3]$

<u>XY Card</u>		<u>X-Y Series Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTA X	0	Dummy values.
4	DELTA Y	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

I.9. File 9: 1-D river/stream transport file (.1tp file)

<u>Value</u>	<u>Description</u>
WMS1TP	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>OP Card</u>	<u>Run option parameters</u>
<u>Field</u> <u>Variable</u>	<u>Value</u> <u>Description</u>
C 1-2 IC1	OP Card group identifier.
C 3 IC3	1 Simulation selection.
1 IDCHEM	Index of chemical transport simulation.
	0 Chemical transport is not simulated.
	1 Chemical transport is simulated.
2 IDSED	Index of sediment transport simulation.
	0 Sediment transport is not simulated.
	1 Sediment transport is simulated.

<u>Field</u> <u>Variable</u>	<u>Value</u> <u>Description</u>
C 1-2 IC1	OP Card group identifier.
C 3 IC3	2 Solver specification.
1 ILUMPT	Index of using mass lumping for transport simulations.
	0 No mass lumping.
	1 Mass lumping.
2 IPNTST	Index of using linear matrix solver for transport simulations.
	1 The pointwise iterative matrix solver.
	2 Preconditioned Conjugate Gradient Method (polynomial),
	3 Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3 IQUART	Index of using quadrature for numerical integration.
	1 Nodal quadrature for line element integration.
	2 Gaussian quadrature for line element integration.
4 IADAPT	Index of using adapted implicit-explicit scheme for the predictor step.
	0 No.
	1 Yes.

<u>Field</u> <u>Variable</u>	<u>Value</u> <u>Description</u>
C 1-2 IC1	OP Card group identifier.
C 3 IC3	3 Weighting factor for transport simulations.
1 WT	Time derivative weighting factor for transport simulation.
	0.5 Crank-Nicolson central.
	1.0 Backward difference.
2 OMET	Relaxation parameter for solving nonlinear matrix equations.
	0.0-1.0 Under relaxation.
	1.0 Exact relaxation.
	1.0-2.0 Over relaxation.
3 OMIT	Relaxation parameter for solving linearized matrix equation.
	0.0-1.0 Under relaxation.
	1.0 Exact relaxation.
	1.0-2.0 Over relaxation.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGENT	0	GGT will not be read.
		1	GGT will be read.
2	GGT	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

IP Card

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	NNITERT
2	NPITER
3	TOLBC
4	TOLBS

Iteration Parameters

<u>Value</u>	<u>Description</u>
IP	Card group identifier.
1	Total simulation time.
+	Allowed number for the non-linear iteration.
+	Allowed number for the linearized iteration.
+	Allowed relative error for getting convergent transport solutions for both dissolved and particulate chemicals.
+	Allowed relative error for getting convergent transport solutions for sediments.

PT Card

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	NXWT
2	IDETQT

Particle tracking parameters

<u>Value</u>	<u>Description</u>
PT	Card group identifier.
1	Particle tracking controlling parameters.
+	Subelement number used in the X-direction in the "in-element" particle tracking.
	Index of particle tracking approach.
1	Using the average-velocity approach.
2	Using the constant-velocity approach.

MP Card

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	i
2	PROPT(1,i)
3	PROPT(2,i)

Material property parameters

<u>Value</u>	<u>Description</u>
MP	Card group identifier.
1	Material property for transport.
+	id of material type.
+	Longitudinal dispersivity associated with the material type [L].
+	Pure diffusion coefficient associated with the material type [L ² /T].

SS card

<u>Field</u>	<u>Variable</u>
C 1-2	IC1
C 3	IC3
1	NP
2	j
3	ITSR(NP,j)

Source/sink parameters

<u>Value</u>	<u>Description</u>
SS	Card group identifier.
1	Source/sink profile for dissolved chemicals.
+	id of global node.
+	id of dissolved chemical.
+	id of xy series to describe the time-dependent source/sink profile for the dissolved chemical at the global node.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	SS	Card group identifier.

C 3	IC3	2	Source/sink profile for suspended sediment.
1	NP	+	id of global node.
2	j	+	id of suspended sediment size.
3	NCHEM	+	Number of dissolved chemicals.
4	ITSR(NP,m)	+	id of xy series to describe the time-dependent source/sink profile for the suspended sediment size at the global node, where $m = NCHEM + j$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	3	Source/sink profile for particulate chemicals on suspended sediments.
1	NP	+	id of global node.
2	j	+	id of suspended sediment.
3	k	+	id of particulate chemical.
4	NCHEM	+	Number of dissolved chemicals.
5	NSSIZE	+	Number of sediment sizes.
6	ITSR(NP,m)	+	id of xy series to describe the time-dependent source/sink profile for the particulate chemical on the suspended sediment size at the global node, where $m = NCHEM + NSSIZE + (j-1)*NCHEM + k$, $j \in [1, NSSIZE]$, and $k \in [1, NCHEM]$.

<u>UB Card</u>		<u>User-specified boundary parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	UB	Card group identifier.
C 3	IC3	1	User-specified boundary conditions for dissolved chemicals.
1	NP	+	id of user-specified boundary node.
2	NPDBT(NP,1)	+	id of global node corresponding to the user-specified boundary node.
3	NPDBT(NP,2)		Index of boundary condition type for the user-specified boundary node.
		1	This is a Dirichlet boundary node with the time-dependent concentration specified.
		2	This is a Variable boundary node with the time-dependent concentration specified if the flow is incoming.
		3	This is a Cauchy boundary node with the time-dependent Cauchy flux specified.
		4	This is a Neumann boundary node with the time-dependent Neumann flux specified.
4	i	+	id of dissolved Chemical.
5	IDTYPT(NP,i)	+	id of xy series to describe the time-dependent profile associated with the user-specified boundary node for the dissolved chemical. It is (1) a concentration profile when NPDB(j,2) = 1. (2) a concentration profile when NPDB(j,2) = 2. (3) a Cauchy flux profile when NPDB(j,2) = 3. (4) a Neumann flux profile when NPDB(j,2) = 4.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	UB	Card group identifier.
C 3	IC3	2	User-specified boundary conditions for suspended sediments.
1	NP	+	id of user-specified boundary node.
2	NPDBT(NP,1)	+	id of global node corresponding to the user-specified boundary node.

3	NPDBT(NP,2)		Index of boundary condition type for the user-specified boundary node.
		1	This is a Dirichlet boundary node with the time-dependent concentration specified.
		2	This is a Variable boundary node with the time-dependent concentration specified if the flow is incoming.
		3	This is a Cauchy boundary node with the time-dependent Cauchy flux specified.
		4	This is a Neumann boundary node with the time-dependent Neumann flux specified.
4	k	+	id of suspended sediment size.
5	NCHEM	+	Number of dissolved chemicals.
6	IDTYPT(NP,i)	+	id of xy series to describe the time-dependent profile associated with the user-specified boundary node for the suspended sediment, <i>where i = NCHEM+k</i> . It is
			(1) a concentration profile when NPDBT(j,2) = 1.
			(2) a concentration profile when NPDBT(j,2) = 2.
			(3) a Cauchy flux profile when NPDBT(j,2) = 3.
			(4) a Neumann flux profile when NPDBT(j,2) = 4.

Field	Variable	Value	Description
C 1-2	IC1	UB	Card group identifier.
C 3	IC3	3	User-specified boundary conditions for particulate chemicals on suspended sediments.
1	NP	+	id of user-specified boundary node.
2	NPDBT(NP,1)	+	id of global node corresponding to the user-specified boundary node.
3	NPDBT(NP,2)		Index of boundary condition type for the user-specified boundary node.
		1	This is a Dirichlet boundary node with the time-dependent concentration specified.
		2	This is a Variable boundary node with the time-dependent concentration specified if the flow is incoming.
		3	This is a Cauchy boundary node with the time-dependent Cauchy flux specified.
		4	This is a Neumann boundary node with the time-dependent Neumann flux specified.
4	j	+	id of suspended sediment size.
5	k	+	id of particulate chemical.
6	NCHEM	+	Number of dissolved chemicals.
7	NSSIZE	+	Number of sediment sizes.
8	IDTYPT(NP,i)	+	id of xy series to describe the time-dependent profile associated with the user-specified boundary node for the particulate chemical on the suspended sediment, <i>where i = NCHEM + NSSIZE + (j-1)*NCHEM + k, j ∈ [1,NSSIZE], and k ∈ [1, NCHEM]</i> . It is
			(1) a concentration profile when NPDBT(j,2) = 1.
			(2) a concentration profile when NPDBT(j,2) = 2.
			(3) a Cauchy flux profile when NPDBT(j,2) = 3.
			(4) a Neumann flux profile when NPDBT(j,2) = 4.

RS card

Rainfall source parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RS	Card group identifier.
C 3	IC3	1	Rainfall source profile for dissolved chemicals.

1st line includes two records as follows.

1	M	+	id of 1-D element.
2	NCHEM	+	Number of dissolved chemicals.

2nd line includes NCHEM records as follows.

1	IRC(M,1)	+	id of xy series to describe the time-dependent concentration profile for the 1 st dissolved chemical in the rainfall that falls on the M th 1-D element.
2	IRC(M,2)	+	id of xy series to describe the time-dependent concentration profile for the 2 nd dissolved chemical in the rainfall that falls on the M th 1-D element.

Up to for the NCHEMth dissolved chemical on the Mth 1-D element.

<u>IC card</u>		<u>Initial condition parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	1	Initial condition parameters.
1	IDCONC		id of initial concentrations.
		0	constant initial concentrations.
		1	variable initial concentrations.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	2	Initially constant conditions for dissolved chemicals
1	j	+	id of the dissolved chemical being input.
2	CCONST(j)	+	Specified initial concentration for the dissolved chemical [M/L ³].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	3	Initially constant conditions for particulate chemicals on suspended sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the suspended sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	CCONST(k)	+	Specified initial concentration for the particulate chemical on suspended sediment being input, where $k = i*NCHEM + j$ [M/L ³].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	4	Initially constant conditions for particulate chemicals on bed sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the bed sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	NSSIZE	+	Number of sediment sizes.
5	CCONST(k)	+	Specified initial concentration for the particulate chemical on

the bed sediment being input, where $k = (i + \text{NSSIZE}) * \text{NCHEM} + j$ [M/L³].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	5	Initially constant conditions for suspended sediments.
1	i	+	id of the suspended sediment size being input.
2	SCONST(i)	+	Specified initial concentration for the suspended sediment of the i th size [M/L ³].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	6	Initially constant conditions for bed sediments.
1	i	+	id of the bed sediment size being input.
2	NSSIZE	+	Number of sediment sizes.
3	SCONST(k)	+	Specified initial concentration for the bed sediment of the i th size, where $k = \text{NSSIZE} + i$ [M/L ³].

<u>XY Card</u>		<u>X-Y Series Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTA X	0	Dummy values.
4	DELTA Y	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

I.10. File 10: 1-D/2-D/3-D chemistry/sediment file (.che file)

<u>Value</u>	<u>Description</u>
WMSCHE	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>RX card</u>		<u>Chemical reaction parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RX	Card group identifier.

C 3	IC3	1	Numbers of reactions and chemicals
1	NRXN	+	Number of reactions.
2	NCHEM	+	Number of dissolved chemicals in 1-D/2-D/3-D systems.
3	NRXNS	+	Number of adsorption reactions in the subsurface.
4	NSITE	+	Number of adsorbing site in the subsurface.
5	NSORB	+	Number of adsorbed chemicals in the subsurface.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	2	Chemical names
1	NCHEM	+	Number of dissolved Chemical.

Note: NCHEM new lines are needed.

(Each line contains the following data: I5,5X,A20)

1	J	+	id of the dissolved chemical being input.
2	CHEMN(J)	+	Name of the J th dissolved chemical.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	3	Adsorbing site names
1	NSITE	+	Number of adsorbing sites.

Note: NSITE new lines are needed.

(Each line contains the following data: I5,5X,A20)

1	J	+	id of the dissolved chemical being input.
2	ASITEN(J)	+	Name of the J th adsorbing site.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	4	Adsorbed chemical names
1	NSORB	+	Number of adsorbed chemicals.

Note: NSORB new lines are needed.

(Each line contains the following data: I5,5X,A20)

1	J	+	id of the dissolved chemical being input.
2.	ASORBN(J)	+	Name of the J th adsorbed chemical.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	5	Reaction rate constants and stoichiometry for aqueous complexation reactions in 1-D/2-D/3-D systems.
1	j	+	id of aqueous complexation reaction.
2	NCHEM	+	Number of dissolved chemicals.
3	FKRX(j)	+	Forward reaction rate constant of the reaction. [reaction dependent]
4	BKRX(j)	+	Backward reaction rate constant of the reaction. [reaction dependent]

Note: Two new lines are needed.

(the first new line)

1	NURTS(j,1)	+	Stoichiometric coefficient of the 1 st dissolved chemical (on the reactant side) in the reaction.
2	NURTS(j,2)	+	Stoichiometric coefficient of the 2 nd dissolved chemical (on the reactant side) in the reaction.

Up to NURTS(j,NCHEM)
(the second new line)

1	NUPDS(j,1)	+	Stoichiometric coefficient of the 1 st dissolved chemical (on the product side) in the reaction.
2	NUPDS(j,2)	+	Stoichiometric coefficient of the 2 nd dissolved chemical (on the product side) in the reaction.

Up to NUPDS(j,NCHEM)

Field	Variable	Value	Description
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	6	Reaction rate constants and stoichiometry for adsorption reactions in the 3-D subsurface system.
1	j	+	id of adsorption reaction.
2	NCHEM	+	Number of dissolved chemicals.
3	NSITE	+	Number of adsorbing sites in the subsurface.
4	NSORB	+	Number of adsorbed chemicals in the subsurface.
5	FKRXSS(j)	+	Forward reaction rate constant of the reaction. [reaction dependent]
6	BKRXSS(j)	+	Backward reaction rate constant of the reaction. [reaction dependent]

Note: Two new lines are needed.

(the first new line)

1	NURTSS(j,1)	+	Stoichiometric coefficient of the 1 st dissolved chemical (on the reactant side) in the reaction.
2	NURTSS(j,2)	+	Stoichiometric coefficient of the 2 nd dissolved chemical (on the reactant side) in the reaction.
	NURTSS(j,NCHEM)		Stoichiometric coefficient of the NCHEM th dissolved chemical (on the reactant side) in the reaction.
	NURTSS(j,NCHEM+1)		Stoichiometric coefficient of the 1 st adsorbing site (on the reactant side) in the reaction.
	NURTSS(j,NCHEM+NSITE)		Stoichiometric coefficient of the NSITE th adsorbing site (on the reactant side) in the reaction.
	NURTSS(j,NCHEM+NSITE+1)		Stoichiometric coefficient of the 1 st adsorbed chemical (on the reactant side) in the reaction.

up to NURTSS(j,NCHEM+NSITE+NSORB)

(the second new line)

1	NUPDSS(j,1)	+	Stoichiometric coefficient of the 1 st dissolved chemical (on the product side) in the reaction.
2	NUPDSS(j,2)	+	Stoichiometric coefficient of the 2 nd dissolved chemical (on the product side) in the reaction.
	NUPDSS(j,NCHEM)		Stoichiometric coefficient of the NCHEM th dissolved chemical (on the product side) in the reaction.

NUPDSS(j,NCHEM+1)	Stoichiometric coefficient of the 1 st adsorbing site (on the product side) in the reaction.
NUPDSS(j,NCHEM+NSITE)	Stoichiometric coefficient of the NSITE th adsorbing site (on the product side) in the reaction.
NUPDSS(j,NCHEM+NSITE+1)	Stoichiometric coefficient of the 1 st adsorbed chemical (on the product side) in the reaction.
up to NUPDS(j,NCHEM+NSITE+NSORB)	

ST card

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	1	Number of sediment sizes
1	NSSIZE	+	Number of sediment sizes.

Sediment parameters

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	2	Parameter associated with each sediment size.
1	j	+	id of Sediment size.
2	SPARA(j,1)		The type of the sediment size.
		1	Cohesive sediment, e.g., clay and silt.
		2	Non-cohesive sediment, e.g., sand.
3	SPARA(j,2)	+	Settling speed of the sediment size [L/T] .
4	SPARA(j,3)	+	Critical shear stress for deposition of the sediment size [M/L/T ²] .
5	SPARA(j,4)	+	Critical shear stress for erosion of the j th size fraction of sediment [M/L/T ²].
6	SPARA(j,5)	+	Erodibility of the sediment size [M/L ²].
7	SPARA(j,6)	+	Specific weight of the sediment size [M/L ³].
8	SPARA(j,7)	+	Median diameter of particles in mixture of the sediment size [L].
9	SPARA(j,8)	+	Critical bottom shear stress of the sediment size at which sediment movement begins [M/L/T ²].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	3	Sorption rate constants and stoichiometry related to suspended sediment.
1	j	+	id of suspended sediment size.
2	i	+	id of dissolved chemical.
3	FKSPSS(j,i)	+	Forward rate constant of the sorption of i th dissolved chemical onto the suspended sediment of the j th size [L ³ /M/T].
4	BKSPSS(j,i)	+	Backward rate constant of the sorption of i th dissolved chemical onto the suspended sediment of the j th size [1/T].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	4	Sorption rate constants and stoichiometry related to bed sediment.
1	j	+	id of bed sediment size.

2	i	+	id of dissolved chemical.
3	FKSPBS(j,i)	+	Forward rate constant of the sorption of i^{th} dissolved chemical onto the bed sediment of the j^{th} size [$L^3/M/T$].
4	BKSPBS(j,i)	+	Backward rate constant of the sorption of i^{th} dissolved chemical onto the bed sediment of the j^{th} size [$1/T$].

VO card

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	VO	Card group identifier.
C 3	IC3	1	Volatilization rate constants.
1	j	+	id of dissolved chemical.
2	IAP(j)	+	id of xy series to describe the time-dependent partial atmospheric pressure profile of the dissolved chemical [atm].
3	FKVO(j)	+	Forward volatilization rate constant of the dissolved chemical [$1/T$].
4	BKVO(j)	+	Backward volatilization rate constant of the dissolved chemical [$M/atm/L^3/T$].

1st order decay parameters

DY card

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	1	Decay constants of dissolved chemicals.
1	j	+	id of dissolved chemical.
2	DCY(j)	+	1 st order decay constant of the dissolved chemical [$1/T$].

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	2	Decay constants of particulate chemicals on suspended sediments.
1	j	+	id of sediment size.
2	i	+	id of particulate chemical.
3	NCHEM	+	Number of dissolved chemicals.
4	DCY(k)	+	Decay constant of the particulate chemical on the suspended sediment [$1/T$]. Where $k = NCHEM \times j + i$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	3	Decay constants of particulate chemicals on bed sediments.
1	j	+	id of sediment size.
2	i	+	id of particulate chemical.
3	NCHEM	+	Number of dissolved chemicals.
4	NSSIZE	+	Number of sediment sizes.
5	DCY(k)	+	Decay constant of the particulate chemical on the bed sediment [$1/T$]. Where $k = NCHEM \times (j + NSSIZE) + i$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	4	Decay constants of adsorbing sites in the subsurface.
1	j	+	id of adsorbing site.
2	NCHEM	+	Number of dissolved chemicals.

3	NSSIZE	+	Number of sediment sizes.
4	DCY(k)	+	Decay constant of the adsorbing site in the subsurface [1/T]. Where $k = NCHEM \times (2 \times NSSIZE + 1) + j$.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	5	Decay constants of adsorbed chemicals in the subsurface.
1	j	+	id of adsorbed chemical.
2	NCHEM	+	Number of dissolved chemicals.
3	NSSIZE	+	Number of sediment sizes.
4	NSITE	+	Number of adsorbing sites in the subsurface.
5	DCY(k)	+	Decay constant of the adsorbed chemical in the subsurface [1/T]. Where $k = NCHEM \times (2 \times NSSIZE + 1) + NSITE + j$.

<u>XY Card</u>		<u>X-Y Series Parameters</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTA X	0	Dummy values.
4	DELTA Y	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

I.11. File 11: 1-D/2-D/3-D mapping file (.map files)

<u>Value</u>	<u>Description</u>
WMSMAP	File type identifier

<u>T1-T3 Cards</u>	<u>Job title</u>
	Only one T1, T2, and T3 card can be used.

<u>CO Card</u>		<u>Mapping information</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	CO	Card group identifier.
C 3	IC3	1	River/stream-related overland nodes
1	N	+	id of global river/stream node.
2	NP12(N)	+	id of the global overland node that is associated with the global river/stream

3	NPS12(1,N)	+	node. This overland node will be excluded in overland simulations. id of the global overland node that serves as the 1 st overland node next to the global river/stream node. This overland node is treated as a boundary node or overland simulations.
f			
4	NPS12(2,N)	+	id of the global overland node that serves as the 2 nd overland node next to the global river/stream node. This overland node is treated as a boundary node for overland simulations.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	CO	Card group identifier.
C 3	IC3	2	Overland-related subsurface nodes
1	N	+	id of global overland node.
2	NP23(N)	+	id of the global subsurface node that is associated with the global overland node. This subsurface node is located on the top boundary of the subsurface domain.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	CO	Card group identifier.
C 3	IC3	3	Overland-related subsurface elements
1	M	+	id of global overland element.
2	MTOP23(M)	+	id of the global subsurface element that is associated with the global overland element. This subsurface element is located on the top boundary of the subsurface domain.

<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C 1-2	IC1	CO	Card group identifier.
C 3	IC3	4	River/stream-related subsurface nodes.
1	N	+	id of global river/stream node.
2	NNTOP13(N)	+	Number of global subsurface nodes that are associated with the N th global river/stream node.

(new line)

1	NTOP12(N,1)	+	id of the global subsurface node that serves as the 1 st node associated with the N th global river/stream node.
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Up to NTOP13(N,NRTOP(N))

<u>EN Card</u>		<u>End of data control</u>	
<u>Field</u>	<u>Variable</u>	<u>Value</u>	<u>Description</u>
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

Table I.1 lists necessary parts for undergoing different simulations.

Table I.1 Data files required to achieve numerical simulations.

Simulation type	Description	Files required
1	1-D river/stream flow	Files 1 and 4
2	1-D river/stream transport	Files 1, 4, 7, and 10
3	1-D river/stream flow and transport	Files 1, 4, 7, and 10
4	2-D overland flow	Files 2 and 5
5	2-D overland transport	Files 2, 5, 8, and 10
6	2-D overland flow and transport	Files 2, 5, 8, and 10
7	3-D subsurface flow	Files 3 and 6
8	3-D subsurface transport	Files 3, 6, 9, and 10
9	3-D subsurface flow and transport	Files 3, 6, 9, and 10
10	1-D/2-D flow	Files 1, 2, 4, 5, and 11
11	2-D/3-D flow	Files 2, 3, 5, 6, and 11
12	1-D/2-D/3-D flow	Files 1, 2, 3, 4, 5, 6, and 11
13	1-D/2-D flow and transport	Files 1, 2, 4, 5, 7, 8, 10, and 11
14	2-D/3-D flow and transport	Files 2, 3, 5, 6, 8, 9, 10, and 11
15	1-D/2-D/3-D flow and transport	Files 1 through 11

On the next page, we give brief description on the files that should be included in the super files for achieving desired simulations. For any of the above fifteen simulations, one needs to provide three super files: one for 1-D, one for 2-D, and the other one for 3-D. In each super file, the BCFT file is a MUST in order to read in the simulation control index, KMOD. If KMOD is zero, it means there is no simulation for the corresponding dimension and no other files are needed to be included in the super file. If KMOD is not zero, the GEOM file is required. If KMOD equals 2, both the BCTT and CHEM files also need to be included in the super file. If coupling systems are considered (1-D/2-D, 2-D/3-D, or 1-D/2-D/3-D), the COMP file must be contained in the 2-D super file. If variable initial conditions are to be read, more files need to be taken into account in the super files, as stated in the table on the next page.

Index in super files	Disk Unit	Input Data File Type	Input Data File Description
GEOM in 1-D super file	11	ASCII	1-D geometry file
BCFT in 1-D super file	11	ASCII	1-D flow file
BCTT in 1-D super file	11	ASCII	1-D transport file
ICWD in 1-D super file	19	ASCII	1-D initial water depth/stage
ICWD in 1-D super file	18	BINARY	1-D initial water depth/stage
ICQL in 1-D super file	21	ASCII	1-D initial velocity
ICQL in 1-D super file	20	BINARY	1-D initial velocity
ICCN in 1-D super file	13	ASCII	1-D initial concentrations
ICCN in 1-D super file	12	BINARY	1-D initial concentrations
PRTF in 1-D super file	17	ASCII	1-D output
GEOM in 2-D super file	41	ASCII	2-D geometry file
BCFT in 2-D super file	41	ASCII	2-D flow file
BCTT in 2-D super file	41	ASCII	2-D transport file
ICWD in 2-D super file	49	ASCII	2-D initial water depth/stage
ICWD in 2-D super file	48	BINARY	2-D initial water depth/stage
ICQL in 2-D super file	51	ASCII	2-D initial velocity
ICQL in 2-D super file	50	BINARY	2-D initial velocity
ICCN in 2-D super file	43	ASCII	2-D initial concentrations
ICCN in 2-D super file	42	BINARY	2-D initial concentrations
PRTF in 2-D super file	47	ASCII	2-D output
GEOM in 3-D super file	71	ASCII	3-D geometry file
BCFT in 3-D super file	71	ASCII	3-D flow file
BCTT in 3-D super file	71	ASCII	3-D transport file
ICHD in 3-D super file	74	ASCII	3-D initial head
ICHD in 3-D super file	73	BINARY	3-D initial head
ICVL in 3-D super file	78	ASCII	3-D initial velocity
ICVL in 3-D super file	77	BINARY	3-D initial velocity
ICMC in 3-D super file	76	ASCII	3-D initial moisture content
ICMC in 3-D super file	75	BINARY	3-D initial moisture content
ICCN in 3-D super file	80	ASCII	3-D initial concentrations
ICCN in 3-D super file	79	BINARY	3-D initial concentrations
PRTF in 3-D super file	72	ASCII	3-D output
CHEM in 1-D, 2-D, or 3-D super files	11, 41, or 71	ASCII	Chemistry file
COMP in 2-D super file	41	ASCII	1-D/2-D/3-D interface file

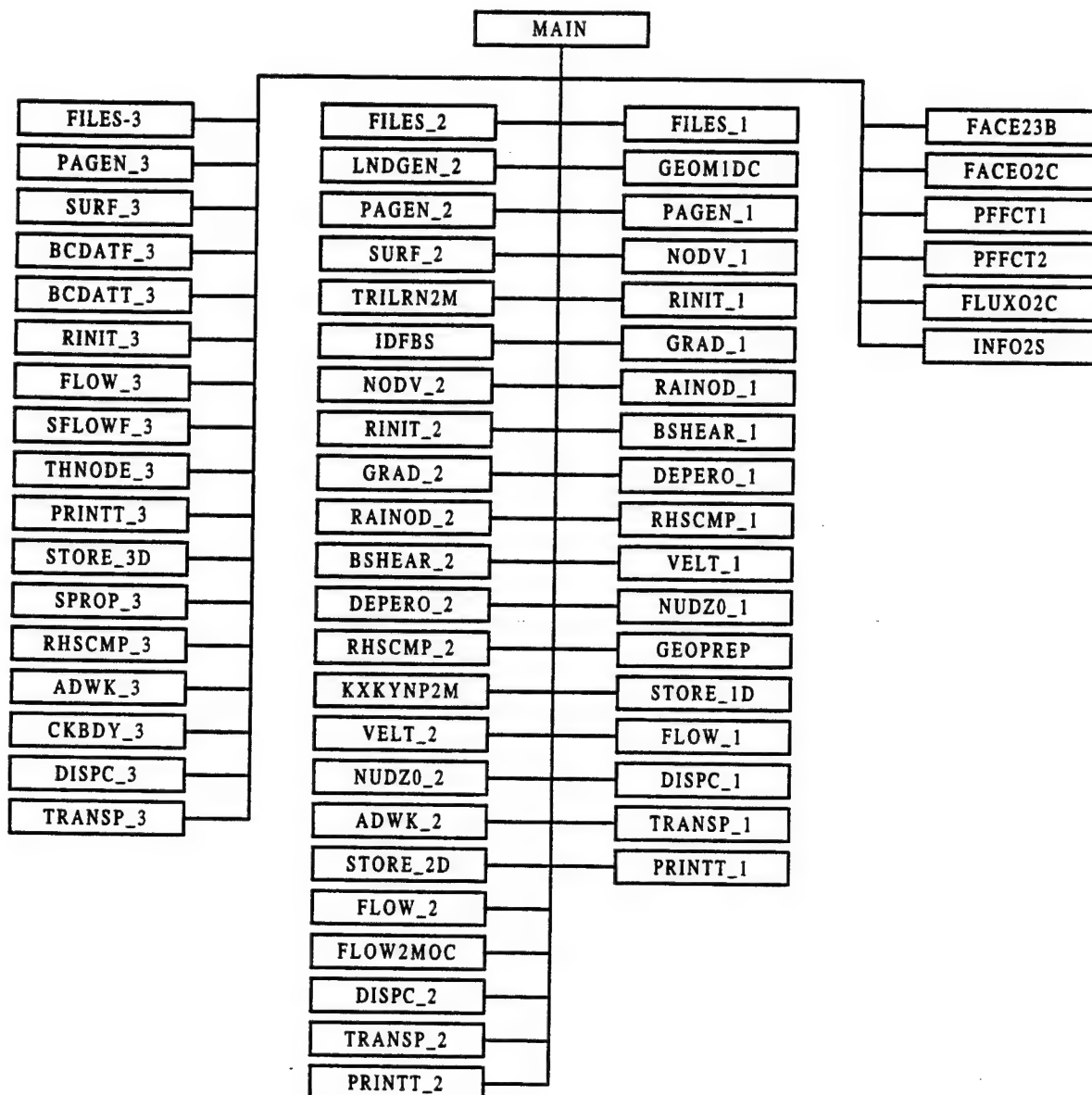
Note: **wms1d.sto**, **wms2d.sto**, and **wms3d.sto** are binary files storing 1-D, 2-D, and 3-D results, respectively, for plotting purposes.

Appendix II. PROGRAM STRUCTURE AND SUBROUTINE DESCRIPTION

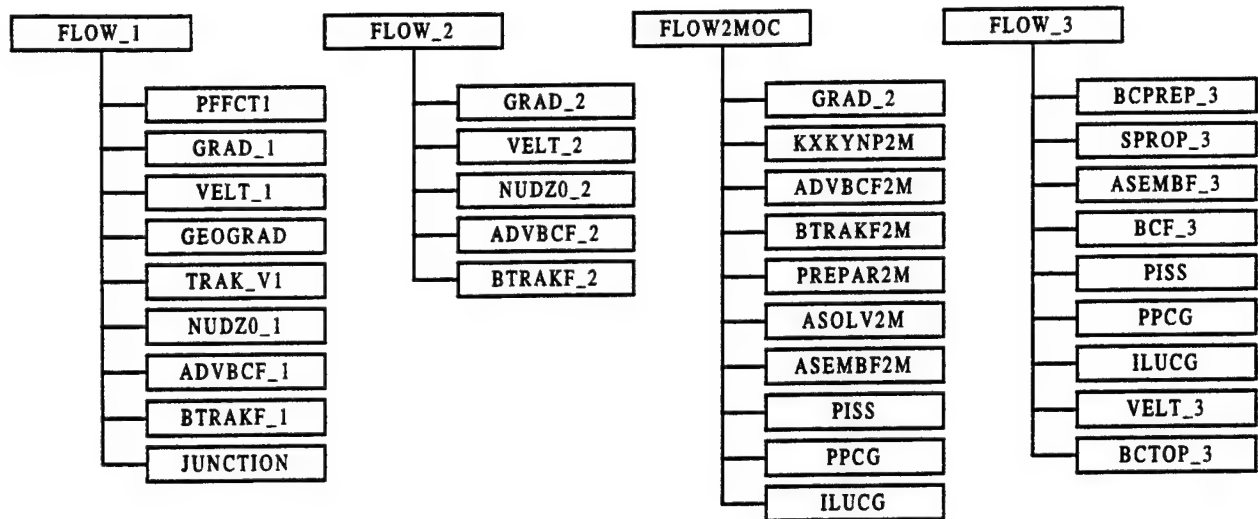
In this appendix, we give plots showing the structure of the computer program and provide description for each subroutine.

II.1. Program structure

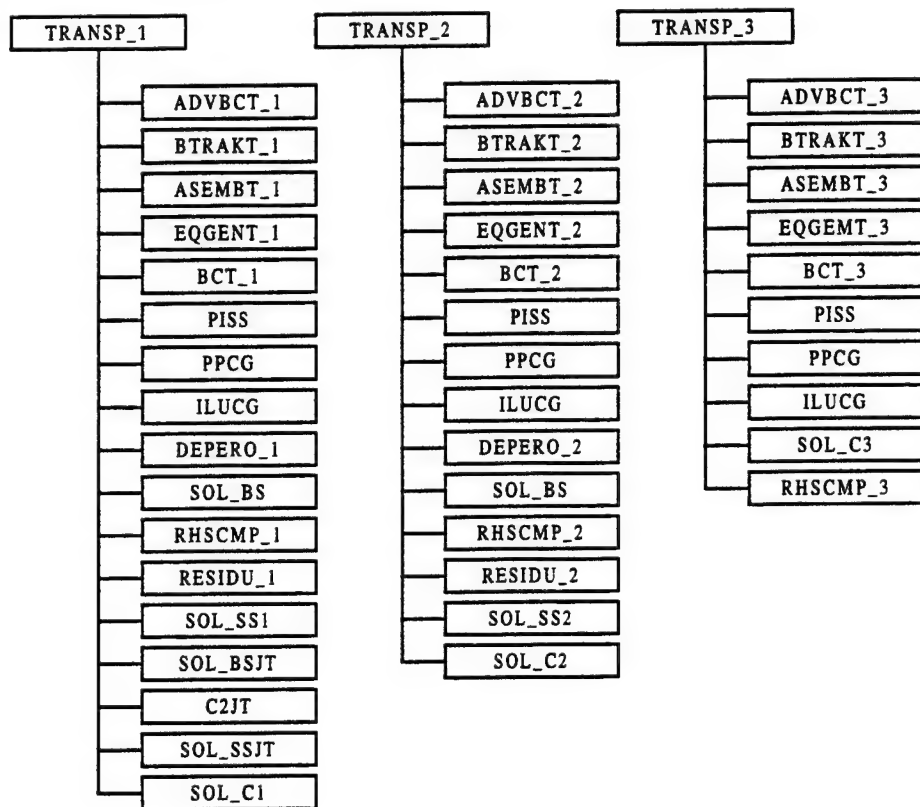
1. Main program and subroutines it calls to.



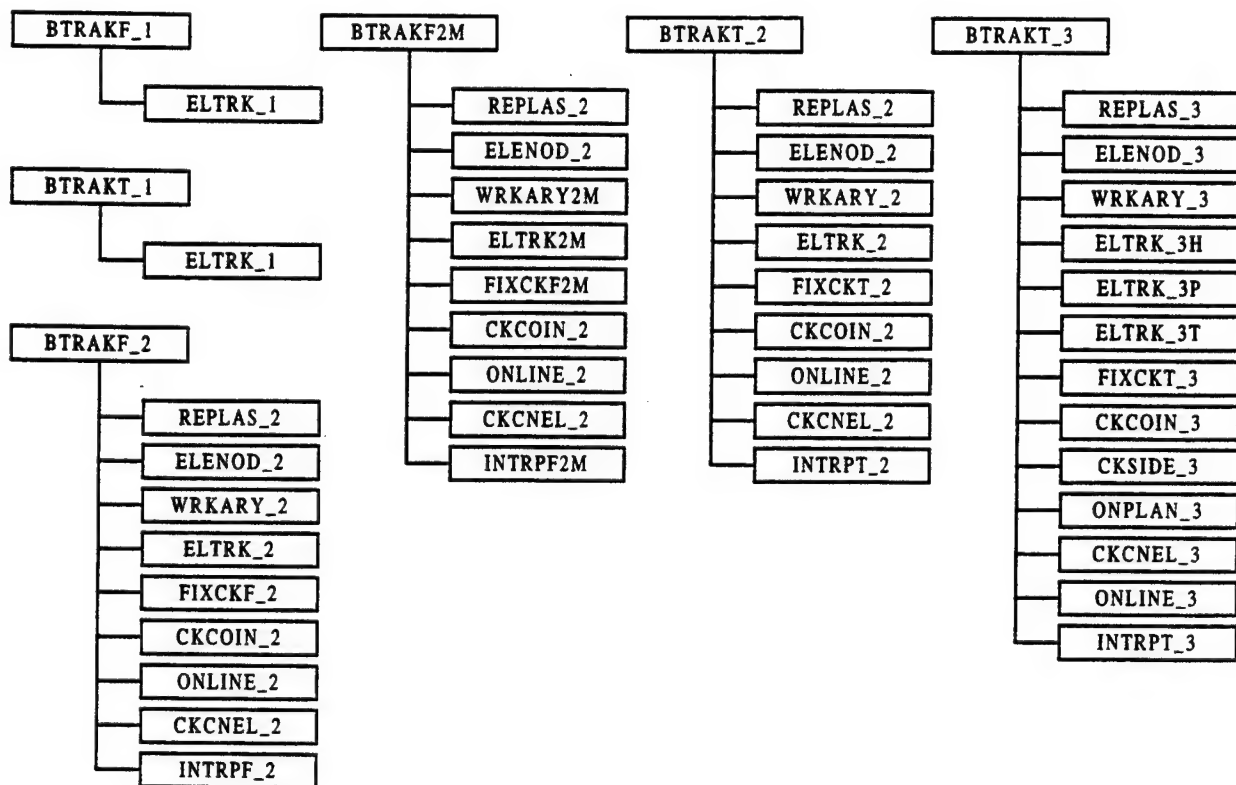
2. Subroutines concerning the computation of water flow.



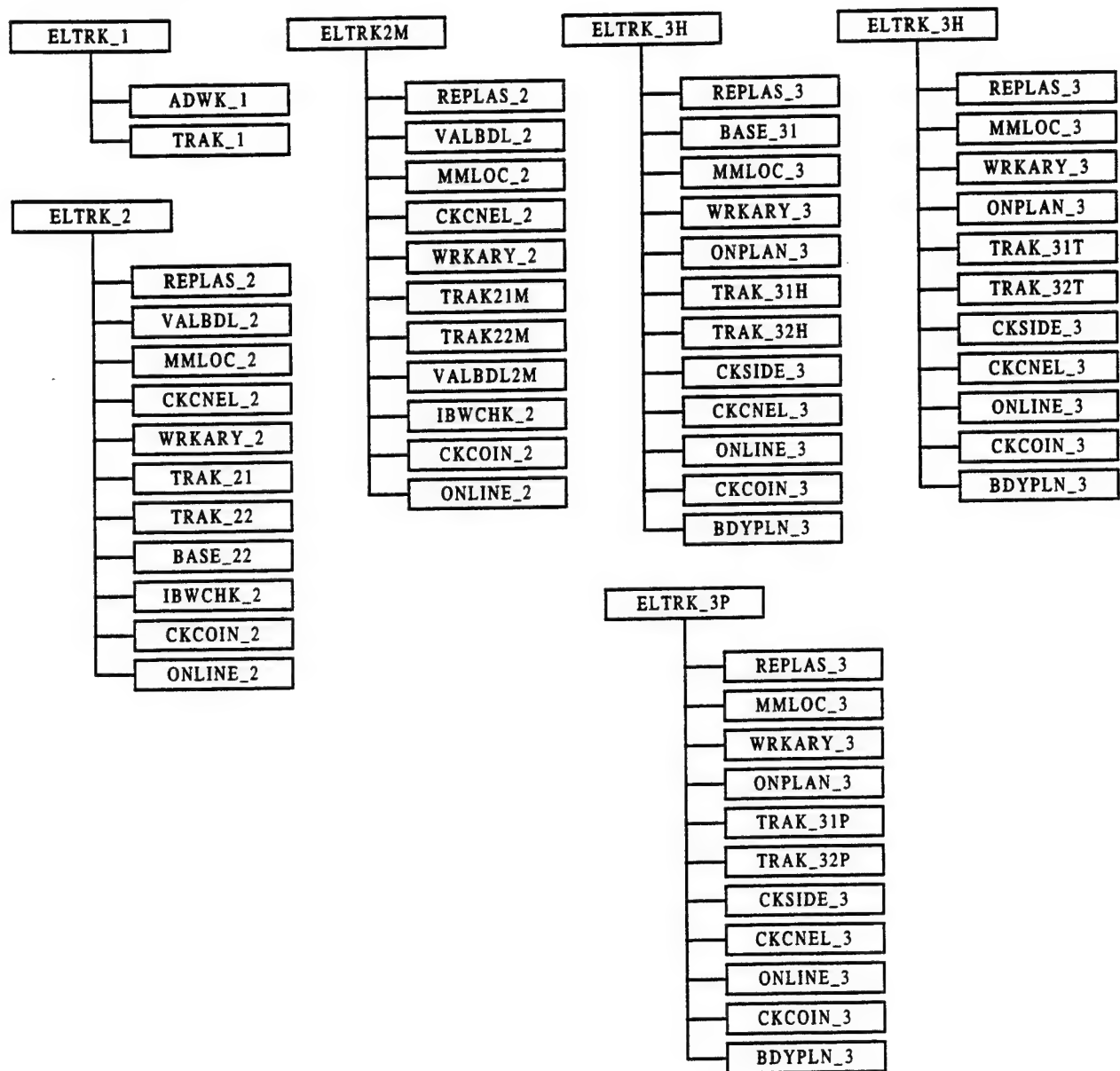
3. Subroutines concerning the computation of chemical/sediment transport.



4. Subroutines concerning backward particle tracking.



5. Subroutines concerning particle tracking in a subelement.



II.2. Subroutine description

MAIN

This main program serves the purpose of controlling the flow path of desired simulations. It calls to Subroutines FILES_3, FILES_2, and FILES_1 to read in necessary data to undergo numerical simulations. It calls to Subroutine FLOW_3 to compute 3-D subsurface flow, Subroutine TRANSP_3 to compute 3-D subsurface chemical transport, Subroutines FLOW_2 or FLOW2MOC to compute 2-D overland flow, Subroutine TRANSP_2 to calculate 2-D overland sediment and chemical transport, Subroutine FLOW_1 to compute 1-D river/stream flow, and Subroutine TRANSP_1 to calculate 1-D river/stream sediment and chemical transport. It also calls to Subroutine INFO2S to evaluate infiltration from overland to subsurface and Subroutine FLUXO2C to estimate both water and material flow rates from overland into river/stream, and vice versa. In addition, it calls to needed subroutines to print or store numerical results, including water depth, stage, discharge, velocity, and concentrations, at desired times.

Subroutine ADVBCF_1

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 1-D flow equations. In this subroutine, boundary conditions with either water depth or upstream inflow specified are implemented to obtain water depth at associated boundary nodes. In addition, Dirichlet-type boundary conditions are applied to junction-connected river/stream nodes.

Subroutine ADVBCF_2

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 2-D flow equations. In this subroutine, boundary conditions with either water depth or upstream inflow specified are implemented to obtain water depth at associated boundary nodes. At the river/stream- and junction-related nodes, the flow direction is from river/stream or junction to the interior of overland, the flux is estimated and the corresponding water depth is calculated accordingly.

Subroutine ADVBCF2M

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 2-D flow equations when the method of characteristics is applied. In this subroutine, boundary conditions with either water stage or upstream inflow specified are implemented to obtain water stage or normal flux, respectively, at associated boundary nodes. At the river/stream- and junction-related nodes, the flow direction is from river/stream or junction to the interior of overland, the normal flux is estimated at the corresponding boundary nodes.

Subroutine ADVBCT_1

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 1-D transport equations of (1) suspended sediment, (2) dissolved chemicals, and (3) particulate chemicals on suspended sediments. Since the diffusive flux is neglected in the Lagrangian Step, only are Dirichlet, Cauchy, and variable boundary conditions are applied. In addition, Dirichlet-type boundary conditions are applied to junction-connected river/stream nodes.

Subroutine ADVBCT_2

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 2-D transport equations of (1) suspended sediment, (2) dissolved chemicals, and (3) particulate chemicals on suspended sediments. Since the diffusive flux is neglected in the Lagrangian Step, only are Dirichlet, Cauchy, and variable boundary conditions are applied. In addition, Variable-type boundary

conditions are applied to river/stream- and junction-related overland nodes if flow direction is determined from river/stream/junction to overland.

Subroutine ADVBCT_3

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 3-D transport equations of dissolved chemicals. Since the diffusive flux is neglected in the Lagrangian Step, only are Dirichlet, Cauchy, and variable boundary conditions are applied. In addition, Variable-type boundary conditions are applied to overland-associated subsurface nodes if flow direction is determined from overland to subsurface.

Subroutine ADWK_1

This subroutine is to determine the working arrays of coordinates (XW) and velocities (VXW) in the element being considered in order to perform the 1-D "in-element" particle tracking.

Subroutine ADWK_2

This subroutine is to determine the working arrays of coordinates (XW), velocities (VXW), subelement indices (IEW), subelement boundary index (IBW), and subelement connectivity (NLRLW and LRLW) in the element being considered in order to perform the 2-D "in-element" particle tracking.

Subroutine ADWK_3

This subroutine is to determine the working arrays of coordinates (XW), velocities (VXW), subelement indices (IEW), subelement boundary index (IBW), and subelement connectivity (NLRLW and LRLW) in the element being considered in order to perform the 3-D "in-element" particle tracking.

Subroutine ALGBY_2

This subroutine is to achieve particle tracking along the 2-D unspecified boundary. Water flow is considered parallel to the boundary on the specified boundary. This subroutine also considers the first-order growth/decay term along characteristics.

Subroutine ALGBYF2M

This subroutine is to achieve particle tracking along the 2-D unspecified boundary. Water flow is considered parallel to the boundary on the specified boundary. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine ALGBY_3

This subroutine is to achieve particle tracking along the 3-D unspecified boundary. Water flow is considered parallel to the boundary on the specified boundary.

Subroutine AREA

This subroutine is to compute the area of a 2-D element, either quadrilateral or triangular.

Subroutine ASEMBF2M

This subroutine is to compose the global matrix equation to adjust 2-D velocity in the last part of the method of characteristic approach when eddy viscosity is taken into account.

Subroutine ASEMBF_3

This subroutine is to compose the global matrix equation to compute pressure head distribution over the domain of interest at the time being considered.

Subroutine ASEMBT_1

This subroutine is to compute global coefficient matrices CMATRX1 and CMATRX2 for 1-D transport equations. CMATRX1 is a mass matrices that takes into account the total time derivative term, while CMATRX2 is stiffness matrices that considers the dispersion term.

Subroutine ASEMBT_2

This subroutine is to compute global coefficient matrices CMATRX1 and CMATRX2 for 2-D transport equations. CMATRX1 is a mass matrices that takes into account the total time derivative term, while CMATRX2 is stiffness matrices that considers the dispersion term.

Subroutine ASEMBT_3

This subroutine is to compute global coefficient matrices CMATRX1 and CMATRX2 for 3-D transport equations. CMATRX1 is a mass matrices that takes into account the total time derivative term, while CMATRX2 is stiffness matrices that considers the dispersion term.

Subroutine ASOLV2M

This subroutine is to construct and solve a set of three algebraic equations (Eqs. (3.129) through (3.131)) that is formed by using the method of characteristics to solve the dynamic wave model.

Subroutine BANSOL

This subroutine is to solver matrix equations with a direct band solver. When the first argument is set to 1, the subroutine triangularizes the band coefficient matrices. When the argument is set to 2, the subroutine solves for the solution (back substitution).

Subroutine BASE_21

This subroutine is to compute the shape functions and their derivatives at a point located in a quadrilateral element, given the local coordinates at the point.

Subroutine BASE_22

This subroutine is to compute the shape functions at a point located in a 2-D element (either triangular or quadrilateral), given the Cartesian coordinates both at the point and element nodes.

Subroutine BASE_31

This subroutine is to compute the shape at a point located in a hexahedral element, given the local coordinates at the point.

Subroutine BASE_32

This subroutine is to compute the shape functions and their derivatives at a point located in a 3-D element (hexahedral, triangular prism, or quadrilateral), given the Cartesian coordinates both at the point and element nodes.

Subroutine BCDATF_3

This subroutine is to transform boundary condition arrays, which are used to implementing 3-D subsurface flow boundary conditions, from containing global nodes to containing boundary nodes.

Subroutine BCDATT_3

This subroutine is to transform boundary condition arrays, which are used to implementing 3-D subsurface transport boundary conditions, from containing global nodes to containing boundary nodes.

Subroutine BCF_3

This subroutine is to implement Dirichlet, Cauchy, Neumann, Variable, and River boundary conditions in computing 3-D subsurface flow. The detailed description for this subroutine can be found elsewhere [Yeh et al, 1997].

Subroutine BCPREP_3

This subroutine is to prepare boundary conditions for the boundary that allows water to flow through it but does not have the flow direction known a priori (i.e., the so-called Variable boundary). The detailed description for this subroutine can be found elsewhere [Yeh et al, 1997].

Subroutine BCTOP_3

This subroutine is to determine which type of boundary condition, flux type or Dirichlet type, is to be applied to the surface/subsurface interface boundary. The criteria involved in this subroutine for determination are similar to those employed in Subroutine BCPREP_3. The detailed description for this subroutine can be found elsewhere [Yeh et al, 1997].

Subroutine BCT_1

This subroutine is to implement boundary conditions, including Dirichlet, Cauchy, Neumann, conventional variable, and junction-related variable types, for 1-D river/stream transport. All boundary conditions, except for the junction-related variable type, are specified at boundary nodes (or reach ends) with time-dependent profiles. For junction-connected nodes, junction-related variable boundary conditions are applied.

Subroutine BCT_2

This subroutine is to implement boundary conditions, including Dirichlet, Cauchy, Neumann, conventional variable, and river/stream-related or junction-related variable types, for 2-D overland transport. Dirichlet boundary conditions are specified at boundary nodes, while the other types of boundary conditions are categorized as flux-type boundary conditions and are specified on boundary sides. Dirichlet, Cauchy, Neumann, and conventional variable boundary conditions are prescribed with time-dependent profiles, while river/stream- or junction-related variable boundary conditions are applied to their associated boundary sides.

Subroutine BCT_3

This subroutine is to implement boundary conditions, including Dirichlet, Cauchy, Neumann, conventional variable, and overland-associated variable types, for 3-D subsurface transport. Dirichlet boundary conditions are specified at boundary nodes, while the other types of boundary conditions are categorized as flux-type boundary conditions and are specified on boundary sides. Dirichlet, Cauchy, Neumann, and conventional variable boundary conditions are prescribed with time-dependent profiles, while overland-associated variable boundary conditions are applied to their associated boundary sides.

Subroutine BDYPLN_3

This subroutine is to locate the four global nodes for returning information to subroutine BTRAKT_3 when the particle has encountered the boundary or working element (i.e., the working element side).

Subroutine BNDRY_3

This subroutine is to determine the location of the target point in a particle tracking along a unspecified boundary side.

Subroutine BSHEAR_1

This subroutine is to achieve the calculation of bottom shear stress at all river/stream nodes.

Subroutine BSHEAR_2

This subroutine is to achieve the calculation of bottom shear stress at all overland nodes.

Subroutine BTRAKF_1

This subroutine is to implement backward particle tracking to obtain the water depth at all 1-D global nodes. Since a first-order approach is used for both kinematic and diffusion models and all source/sink rate terms can be expressed a linear function of water depth, we thus take into account the first-order decay/growth rate along the characteristics when we implement backward particle tracking. As for the zeroth-order source/sink rate, we simply multiply this rate by the time-step size being considered and add the product to the outcome of backward particle tracking.

Subroutine BTRAKF_2

This subroutine is to implement backward particle tracking along three characteristics to obtain the Lagrangian water depth and velocity at all 2-D global nodes when the method of characteristics is used to solve 2-D flow equations. The spatial reachout approach is currently implemented in this subroutine.

Subroutine BTRAKF2M

This subroutine is to implement backward particle tracking to obtain the water depth at all 2-D global nodes. Since a first-order approach is used for both kinematic and diffusion models and all source/sink rate terms can be expressed a linear function of water depth, we thus take into account the first-order decay/growth rate along the characteristics when we implement backward particle tracking. As for the zeroth-order source/sink rate, we simply multiply this rate by the time-step size being considered and add the product to the outcome of backward particle tracking.

Subroutine BTRAKT_1

This subroutine is to implement backward particle tracking to obtain the Lagrangian values of concentrations of (1) dissolved chemicals, (2) suspended sediments, and (3) particulate chemicals on suspended sediments at all 1-D global nodes.

Subroutine BTRAKT_2

This subroutine is to implement backward particle tracking to obtain the Lagrangian values of concentrations of (1) dissolved chemicals, (2) suspended sediments, and (3) particulate chemicals on suspended sediments at all 2-D global nodes.

Subroutine BTRAKT_3

This subroutine is to implement backward particle tracking to obtain the Lagrangian values of concentrations of dissolved chemicals at all 3-D global nodes.

Subroutine CFACE_3

This subroutine is to transform the 3-D element face ID generated from GMS to the convention used in the computer code.

Subroutine CHNGSN

This subroutine is to change sign of the velocities at point P (the starting location), point Q (the ending location), and working subelement nodes in the process of 2-D or 3-D "in-element" particle tracking.

Subroutine CKBDY_3

This subroutine is to determine the unspecified boundary sides that are connected to global nodes. The information is saved in two arrays (IBDY and NBDYB) and is used for implementing particle tracking along the unspecified boundary.

Subroutine CKCNEL_2

This subroutine is to determine the element that connects to a specified element through the element side with the N1-th and N2-th global nodes serving as the two end nodes of the 2-D side.

Subroutine CKCNEL_3

This subroutine is to determine the element that connects to a specified element through the element side with the N1-th and N2-th global nodes serving as the two end nodes of the 3-D side.

Subroutine CKCOIN_2

This subroutine is to determine whether or not a specific node coincides with the N1-th global node or the N2-th global node.

Subroutine CKCOIN_3

This subroutine is to determine whether or not a specific node coincides with the N1-th global node, the N2-th global node, the N3-th global node, or the N4-th global node.

Subroutine CKSIDE_3

This subroutine is to determine whether or not a specific node is on the 3-D element side that has global nodes N1, N2, N3, and N4 as its side nodes.

Subroutine COMAP

This subroutine is to (1) relate 1-D river/stream nodes to 2-D overland nodes, (2) relate 2-D overland nodes to 3-D subsurface nodes, and (3) relate 2-D overland elements to 3-D subsurface elements. Those overland nodes which correspond to river/stream nodes will not be taken into account in 2-D overland simulations.

Subroutine CRACKD

This subroutine is to read real numbers in order from a line data record.

Subroutine CRACKI

This subroutine is to read integer numbers in order from a line data record.

Subroutine C2JT

This subroutine is to compute the flow rate of (1) water (when ID = 1), (2) dissolved chemicals (when ID = 2), (3) particulate chemicals on suspended sediments (when ID = 3), and (4) particulate chemicals on bed sediments (when ID = 4) from junction-connected river/streams to a specified junction.

Subroutine DEPERO_1

This subroutine is to compute the deposition and erosion rates either at a river/stream node (when NP is not zero and J is zero) or at a junction (when NP equals zero and J is not equal to zero). Both cohesive and non-cohesive cases are taken into account. The following equations are used to achieve the computation at a river/stream node.

(1) For cohesive sediments:

$$D_n = V_{sn} S_n \left[1 - \frac{\tau_b}{\tau_{cDn}} \right] \quad (\text{II.1})$$

$$R_n = E_n \left[\frac{\tau_b}{\tau_{cRn}} - 1 \right] \quad (\text{II.2})$$

where V_{sn} is the settling velocity of the n-th size fraction sediment [L/T]; τ_b is the bottom shear stress or the bottom friction stress [M/L/T²]; τ_{cDn} is the critical shear stress for the deposition of the n-th size fraction sediment [M/L/T²]; τ_{cRn} is the critical shear stress for the erosion of the n-th size fraction sediment [M/L/T²]; E_n is the erodibility of the n-th size fraction sediment [M/L²]. In the computer code, V_{sn} , τ_{cDn} , τ_{cRn} , and E_n are input parameters, while τ_b is computed in the flow module. The above two equations can be found from "CHNTRN: A River/stream Transport Model for Simulating Sediment and Chemical Distribution in a Stream/River Network" by Yeh (1983), ORNL-5882 Report, Eq. (29) on page 12.

(2) For non-cohesive sediments:

$$D_n = \frac{G_{sAn} - G_{sn}}{\Delta L} \quad (\text{II.3})$$

$$R_n = \frac{G_{sn} - G_{sAn}}{\Delta L} \quad (\text{II.4})$$

where G_{sAn} is the actual load rate of the n-th size fraction sediment per unit width at a upstream location [M/L/T]; G_{sn} is the maximum load rate (capacity) of the n-th size fraction sediment per unit width at a downstream location [M/L/T]; ΔL is the distance between the upstream and the downstream locations. Eqs. The above two equations can be found from "CHNTRN: A River/stream Transport Model for Simulating Sediment and Chemical Distribution in a Stream/River Network" by Yeh (1983), ORNL-5882 Report, Eq. (30) on page 12. In the computer code, ΔL can be determined based on the coordinates, while G_{sAn} and G_{sn} are computed based on the following equations.

$$G_{sAn} = S_n * u * r \quad (\text{II.5})$$

$$G_{sn} = 10 \frac{\rho^2 u r S (\tau_b - \tau_{cm})}{g d_n (\rho_{sn} - \rho)^2} \quad (\text{II.6})$$

where ρ is the fluid density [M/L³]; ρ_{sn} is the density of the n-th size fraction sediment [M/L³]; u is river/stream flow velocity [L/T]; r is hydraulic radius [L]; S the friction slope, d_n is the median diameter of the n-th size fraction sediment particle [L]; g is gravity [L/T²]; τ_{cm} is the critical bottom shear stress of the n-th size fraction sediment at which sediment movement begins [M/L/T²]. Among these parameters, ρ , ρ_{sn} , d_n , and τ_{cm} are input by users, while u , r , and S are estimated in the flow module. The above equation is from "Hydraulics of Sediment Transport" by Walter Hans Graf (1984), Water Resources Publication, Eq. (7.14) on page 128.

To estimate the deposition and erosion rates at a junction, the following weighted-average equations are employed.

$$D_n(J) = \frac{\sum_{i=1}^{NJRTH(J)} u_i P_i D_{ni}}{\sum_{i=1}^{NJRTH(J)} u_i P_i} \quad (II.7)$$

$$R_n(J) = \frac{\sum_{i=1}^{NJRTH(J)} u_i P_i R_{ni}}{\sum_{i=1}^{NJRTH(J)} u_i P_i} \quad (II.8)$$

where $D_n(J)$ and $R_n(j)$ are the deposition and erosion rate at the J-th junction; u_i , P_i , D_{ni} , R_{ni} are the velocity, wetted perimeter, deposition rate, and erosion rate at the river/stream node that serves as the i-th junction-connected node to the J-th junction; $NJRTH(J)$ is number of river/stream reaches that are connected to the J-th junction.

Subroutine DEPERO_2

This subroutine is to compute the deposition and erosion rates at an overland node. The equations described in Subroutine DEPERO_1 are also used here.

Subroutine DGELG

This subroutine is to solve matrix equations by a direction solver incorporated with full-pivoting.

Subroutine DISPC_1

This subroutine is to compute dispersion coefficients for 1-D transport simulations. The coefficient is evaluated at every quadrature node of elements.

Subroutine DISPC_2

This subroutine is to compute dispersion coefficients for 2-D transport simulations. The coefficient is evaluated at every quadrature node of elements.

Subroutine DISPC_3

This subroutine is to compute dispersion coefficients for 3-D transport simulations. The coefficient is evaluated at every quadrature node of elements.

Function DOTPRD

This function is to compute the inner product of two given vectors.

Subroutine ELENOD_2

This subroutine is to determine the number of element nodes for a specified 2-D element.

Subroutine ELENOD_3

This subroutine is to determine the number of element nodes and the element shape for a specified 3-D element.

Subroutine ELTRK_1

This subroutine is to implement the 1-D "in-element" particle tracking for a particle with its starting location specified. During the tracking process, many elements can be passed through. The first-order growth/decay term is also taken into account in the tracking.

Subroutine ELTRK_2

This subroutine is to implement the 2-D "in-element" particle tracking in a specified element. The first-order growth/decay term is also taken into account in the tracking.

Subroutine ELTRK2M

This subroutine is to implement the 2-D "in-element" particle tracking in a specified element. It is used only when the method of characteristics is used to solve the 2-D flow equation.

Subroutine ELTRK_3H

This subroutine is to implement the 3-D "in-element" particle tracking in a specified hexahedral element.

Subroutine ELTRK_3P

This subroutine is to implement the 3-D "in-element" particle tracking in a specified triangular prism element.

Subroutine ELTRK_3T

This subroutine is to implement the 3-D "in-element" particle tracking in a specified tetrahedral element.

Subroutine EQGENT_1

This subroutine is to generate matrix equations for 1-D transport simulations. When $IDS = 0$, it is for the transport of the IDS -th suspended sediment. When $IDS = 0$, it is for the transport of the IDS -th dissolved chemical. When neither IDS nor IDS equals zero, it is for the IDS -th particulate chemical on the IDS -th suspended sediment.

Subroutine EQGENT_2

This subroutine is to generate matrix equations for 2-D transport simulations. When $IDS = 0$, it is for the transport of the IDS -th suspended sediment. When $IDS = 0$, it is for the transport of the IDS -th dissolved chemical. When neither IDS nor IDS equals zero, it is for the IDS -th particulate chemical on the IDS -th suspended sediment.

Subroutine EQGENT_3

This subroutine is to generate matrix equations for 3-D transport simulations. Only are the dissolved chemicals involved.

Subroutine FACEO2C

This subroutine is to determine those overland boundary sides which are either river/stream-related or junction-related.

Subroutine FACE23B

This subroutine is to prepare arrays for describing the surface/subsurface interface boundary, based on the mapping information from the input data.

Function FCOS_2

This is to determine the direction of the outer product of two 2-D vectors.

Function FCOS_3

This is to determine the direction of the inner product of two 3-D vectors.

Subroutine FILES_1

This subroutine is to read in information in order to perform 1-D river/stream simulations. The information includes (1) geometry data, (2) flow simulation data, and (3) transport simulation data.

Subroutine FILES_2

This subroutine is to read in information in order to perform 2-D overland simulations. The information includes (1) geometry data, (2) flow simulation data, (3) transport simulation data, and (4) 1-D/2-D and 2-D/3-D interface data.

Subroutine FILES_3

This subroutine is to read in information in order to perform 3-D subsurface simulations. The information includes (1) geometry data, (2) flow simulation data, and (3) transport simulation data.

Subroutine FIXCKF_2

This subroutine is to handle the case in the particle tracking of 2-D water flow when a particle encounters the boundary. If this boundary is a specified (flow-through) boundary, the current particle tracking stops here and interpolation is employed to compute the Lagrangian value. If this boundary is unspecified (closed), on the other hand, the flow direction is parallel to the boundary and particle tracking along the boundary proceeds until either the available tracking time is completely consumed or a specified boundary is reached. The first-order growth/decay term is also taken into account in the tracking.

Subroutine FIXCKF2M

This subroutine is to handle the case in the particle tracking of 2-D water flow when a particle encounters the boundary. If this boundary is a specified (flow-through) boundary, the current particle tracking stops here and interpolation is employed to compute the Lagrangian value. If this boundary is unspecified (closed), on the other hand, the flow direction is parallel to the boundary and particle tracking along the boundary proceeds until either the available tracking time is completely consumed or a specified boundary is reached. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine FIXCKT_2

This subroutine is to handle the case in the particle tracking of 2-D chemical transport when a particle encounters the boundary. If this boundary is a specified (flow-through) boundary, the current particle tracking stops here and interpolation is employed to compute the Lagrangian value. If this boundary is unspecified (closed), on the other hand, the flow direction is parallel to the boundary and particle tracking along the boundary proceeds until either the available tracking time is completely consumed or a specified boundary is reached.

Subroutine FIXCKT_3

This subroutine is to handle the case in the particle tracking of 3-D chemical transport when a particle encounters the boundary. If this boundary is a specified (flow-through) boundary, the current particle tracking stops here and interpolation is employed to compute the Lagrangian value. If this boundary

is unspecified (impermeable), on the other hand, the flow direction is parallel to the boundary and particle tracking along the boundary proceeds until either the available tracking time is completely consumed or a specified boundary is reached.

Function FKAPA_2

This function is to compute the bottom friction coefficient, κ , as defined as follows.

$$\kappa = \frac{g n |\nabla(h + Z_o)|^{1/2} [1 + (\nabla Z_o)^2]^{2/3}}{h^{2/3}} \quad (\text{II.9})$$

Subroutine FKK1_1

This subroutine is to compute the flow velocity at global nodes for either the kinematic model or the diffusion model of 1-D river/stream flow.

Subroutine FKK1_2

This subroutine is to compute the flow velocity at global nodes for either the kinematic model or the diffusion model of 2-D overland flow.

Subroutine FKK2_1

This subroutine is to compute the source/sink term at a global node due to non-uniform bed slope or potential slope for the kinematic model or the diffusion model, respectively, of 1-D river/stream flow.

Subroutine FKK2_2

This subroutine is to compute the source/sink term at a global node due to non-uniform bed slope or potential slope for the kinematic model or the diffusion model, respectively, of 2-D overland flow.

Subroutine FLOW_1

This subroutine serves as the control panel of computing 1-D river/stream flow by using the Lagrangian approach to solve the diffusion model. The Picard method is used to deal with nonlinearity. During each nonlinear iteration, the working velocity is first estimated based on the working water depth with Eq. (2.3). This working velocity is then used to achieve backward particle tracking in the Lagrangian approach to obtain the updated water depth. Convergence is determined by checking the maximum relative error of water depth. Relaxation technique is applied to update the working water depth for the next iteration if convergence has not been reached. When junctions exist, water budget is employed to determine the water depth at junctions. The flow rates of water coming from or going into the junction-connected reaches are calculated based on the working velocity and cross-sectional areas at junction-reach interfacial nodes (e.g., Nodes 10, 13, and 32 in Figure 4.4).

Subroutine FLOW_2

This subroutine serves as the control panel of computing 2-D overland flow by using the Lagrangian approach to solve the diffusion model. The Picard method is used to deal with nonlinearity. During each nonlinear iteration, the working velocity is first estimated based on the working water depth with Eqs. (2.12) and (2.13). This working velocity is then used to achieve backward particle tracking in the Lagrangian approach to obtain the updated water depth. Convergence is determined by checking the maximum relative error or water depth. Relaxation technique is applied to update the working water depth for the next iteration if convergence has not been reached.

Subroutine FLOW2MOC

This subroutine serves as the control panel of computing 2-D overland flow by using the method of characteristics to solve the dynamic model. The Picard method is used to deal with nonlinearity. During each nonlinear iteration, The characteristic equation (Eq. (3.85)) is solved first by the backward particle tracking along three characteristics. After H^* , u^* , and v^* are determined, we compute H , u , and v by solving Eqs. (3.151) through (3.153). Convergence is determined by checking the maximum relative error of H , u , and v . Relaxation technique is applied to update the working water stage and velocity for the next iteration if convergence has not been reached.

Subroutine FLOW_3

This subroutine serves as the control panel of computing 3-D subsurface flow by using the Gelarkin finite element method solve the Richard's equation. The Picard method is used to deal with nonlinearity. During each nonlinear iteration, pressure head is computed and moisture content, water capacity, and hydraulic conductivity are updated accordingly. Convergence is determined by checking the maximum absolute error. The detailed description for this subroutine can be found elsewhere [Yeh et al, 1997].

Subroutine FLUXO2C

This subroutine is to compute flow rate of water, dissolved chemicals, suspended sediments, and particulate chemicals on suspended sediments from overland to both river/stream nodes and river/stream junctions. When the outward normal velocity is positive at a river/stream- or junction-related overland boundary node, there is water flowing from overland to the associated river/stream node or junction. If the outward normal velocity is negative, two cases are taken into account: when the associated river/stream/junction water stage is higher than the bottom elevation of this overland boundary node, there is water flowing from river/stream/junction to overland; otherwise, there is no water passing through the 1D-2D interface.

Subroutine FTAUB_1

This subroutine is to calculate bottom shear stress at a river/stream node. The bottom shear stress is computed according to the following equation.

$$\tau^b = u \rho g n |\nabla(h + Z_o)|^{1/2} [1 + (\nabla Z_o)^2]^{2/3} r^{1/3} \quad (\text{II.10})$$

where τ^b is bottom shear stress; u is river/stream velocity; ρ is water density; g is gravity; n is Manning's n ; h is water depth; Z_o is bottom elevation; and r is hydraulic radius.

Subroutine FTAUB_2

This subroutine is to calculate bottom shear stress at an overland node. The bottom shear stress is computed according to the following equations.

$$\tau_x^b = u \rho g n |\nabla(h + Z_o)|^{1/2} [1 + (\nabla Z_o)^2]^{2/3} h^{1/3} \quad (\text{II.11})$$

$$\tau_y^b = v \rho g n |\nabla(h + Z_o)|^{1/2} [1 + (\nabla Z_o)^2]^{2/3} h^{1/3} \quad (\text{II.12})$$

where τ_x^b and τ_y^b are bottom shear stress in x- and y-directions, respectively; u and v are velocity components in x- and y-directions, respectively; ρ is water density; g is gravity; n is Manning's n ; h is water depth; Z_o is bottom elevation.

Subroutine GAUPNT_2

This subroutine is to compute shape functions and their derivatives at quadrature nodes.

Subroutine GEOGRAD

This subroutine is to compute the derivatives of hydraulic radius and average river/stream width with respect to distance and water depth in 1-D river/stream flow simulations.

Subroutine GEOM1DC

This subroutine is to determine the river/stream-associated overland elements that are not to be taken into account in 2-D overland simulations.

Subroutine GEOM_1

This subroutine is to read in 1-D river/stream geometry, including coordinates and element indices.

Subroutine GEOM_2

This subroutine is to read in 2-D overland geometry, including coordinates and element indices.

Subroutine GEOM_3

This subroutine is to read in 3-D subsurface geometry, including coordinates and element indices.

Subroutine GEOPREP

This subroutine is to prepare the profile of describing the derivatives of both hydraulic radius and average river/stream width with respect to water depth, based on the prescribed profiles of river/stream geometry.

Subroutine GRAD_1

This subroutine is to compute the spatial derivatives of water depth, stage, flow velocity, average river/stream width, and Manning's n as desired in 1-D river/stream simulations. In addition, the second spatial derivatives of water depth and stage are calculated as needed.

Subroutine GRAD_2

This subroutine is to compute the spatial derivatives of water depth, stage, flow velocity, and Manning's n as desired in 2-D overland simulations. In addition, the second spatial derivatives of water depth and stage are calculated as needed.

Subroutine IBWCHK_2

This subroutine is to determine the two global nodes that serve as the two end node of an element side. This element side is the side that the particle has encountered when it passes through the element being considered.

Subroutine IDFBFS

This subroutine is to relate flux-type boundary sides with global boundary sides. The relationship is stored in two arrays: one for flow simulations and the other for transport simulations.

Subroutine ILUCG

This subroutine is to solve the linearized matrix equation that is sparse asymmetric with the preconditioned conjugate gradient method using the incomplete Cholesky decomposition as a preconditioner.

Subroutine INFO2S

This subroutine is to compute infiltration flux (L^3/T) at all overland nodes. Based on the concept of continuity of flux, the following equation is used to compute the flux.

$$\Phi_i = \int_R -(\mathbf{n} \cdot \mathbf{V}) \sqrt{1 + \left(\frac{\partial Z_o}{\partial x}\right)^2} \sqrt{1 + \left(\frac{\partial Z_o}{\partial y}\right)^2} dR \quad (\text{II.13})$$

where \mathbf{n} and \mathbf{V} are the outward unit normal vector and Darcy velocity (specific discharge), respectively, at the 3-D subsurface boundary node that is corresponding to the 2-D overland node being considered; $\partial Z_o/\partial x$ and $\partial Z_o/\partial y$ are the derivatives of elevation in the x- and the y-directions, respectively, at the 2-D overland node.

Subroutine INTRPF_2

This subroutine is to determine the Lagrangian water depth by interpolation after backward particle tracking in solving flow governing equations when the diffusion wave model is taken into account.

Subroutine INTRPF2M

This subroutine is to determine the Lagrangian characteristic quantities by interpolation after backward particle tracking in solving flow governing equations when the method of characteristics is used to deal with the dynamic wave model.

Subroutine INTRPT_2

This subroutine is to determine the Lagrangian chemical and suspended sediment concentrations by interpolation after backward particle tracking in the Lagrangian step of solving 2-D transport governing equations.

Subroutine INTRPT_3

This subroutine is to determine the Lagrangian chemical concentrations by interpolation after backward particle tracking in the Lagrangian step of solving 3-D transport governing equations.

Subroutine JACOBI_1

This subroutine is to compute the Jacobian for the chemical system at the NP-th node (when NP is not equal to zero and J equals zero) or the J-th junction (when NP equals zero and J is not equal to zero). The Jacobian elements are defined as follows.

For the case at the NP-th node:

(1) For dissolved chemicals:

$$\frac{\partial \text{RESC}_i}{\partial (C_1^w)^{N+1}} = \delta_{i1} A + \delta_{i2} \delta t \left[\lambda_i^w A + R - I + R_1 + R_2 + A k_{i1}^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} \right] - \delta t \left[\sum_{m=1}^{N_{rx}} k_m^{rb} A b_{mi} (C_1^w)^{b_{mi}-1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{b_{mj}} - \sum_{m=1}^{N_{rx}} k_m^{rf} A a_{mi} (C_1^w)^{a_{mi}-1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{a_{mj}} \right] \quad (\text{II.14})$$

$i \in [1, N_c]$

$$\frac{\partial \text{RESC}_i}{\partial (C_{nl}^s)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sb} S_n A \quad n \in [1, N_s], \quad i \in [1, N_c], \quad (\text{II.15})$$

$$\frac{\partial \text{RESC}_i}{\partial (C_{nl}^b)^{N+1}} = -\delta_{il} \delta t k_{ni}^{bb} M_n P \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (\text{II.16})$$

(2) For particulate chemicals on suspended sediments:

$$\frac{\partial \text{RESC}_k}{\partial (C_1^w)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sf} S_n A \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad (\text{II.17})$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^s)^{N+1}} = \delta_{il} A S_n + \delta_{il} \delta t B D_n + \delta_{il} \delta t S_n \left[\lambda_{ni}^s A + k_{ni}^{sb} A + R - I + R_1 + R_2 \right] \quad (\text{II.18})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^b)^{N+1}} = -\delta_{il} \delta t B R_n \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad (\text{II.19})$$

(3) For particulate chemicals on bed sediments:

$$\frac{\partial \text{RESC}_k}{\partial (C_1^w)^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bf} M_n \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad (\text{II.20})$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^s)^{N+1}} = -\delta_{il} \Delta t D_n \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad (\text{II.21})$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^b)^{N+1}} = \delta_{il} M_n + \delta_{il} \Delta t R_n + \delta_{il} \Delta t M_n \left[\lambda_{ni}^b + k_{ni}^{bb} \right] \quad (\text{II.22})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

It is noted that if SS, R, R1, and R2 are negative (i.e., sinks), they should not appear in Eqs. (II.14) and (II.18). Likewise, if I is positive (i.e., sink), it must not appear in the two equations.

For the case at the J-th junction:

(1) For dissolved chemicals:

$$\frac{\partial \text{RESC}_i}{\partial (C_1^w(J))^{N+1}} = \delta_{il} V(J) + \delta_{il} \Delta t \left[\lambda_i^w V(J) + V(J) k_i^{sf} + \sum_{n=1}^{N_s} S_n(J) V(J) k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n(J) A(J) k_{ni}^{bf} \right] -$$

$$\Delta t \left[\sum_{m=1}^{N_x} k_m^{rb} V(J) b_{ml} (C_1^w(J))^{b_{ml}-1} \prod_{j=1, j \neq l}^{N_c} (C_j^w(J))^{b_{mj}} - \sum_{m=1}^{N_x} k_m^{rf} V(J) a_{ml} (C_1^w(J))^{a_{ml}-1} \prod_{j=1, j \neq l}^{N_c} (C_j^w(J))^{a_{mj}} \right] \quad (\text{II.23})$$

$$i \in [1, N_c]$$

$$\frac{\partial \text{RESC}_i}{\partial (C_{nl}^s(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{sb} S_n(J) V(J) \quad n \in [1, N_s], \quad i \in [1, N_c], \quad (\text{II.24})$$

$$\frac{\partial \text{RESC}_i}{\partial (C_{nl}^b(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bb} M_n(J) A(J) \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (\text{II.25})$$

(2) For particulate chemicals on suspended sediments:

$$\frac{\partial \text{RESC}_k}{\partial (C_1^w(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{sf} S_n(J) V(J) \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad (\text{II.26})$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^s(J))^{N+1}} = \delta_{il} V(J) S_n(J) + \delta_{il} \Delta t A(J) D_n(J) + \delta_{il} \Delta t S_n(J) \left[\lambda_{ni}^s V(J) + k_{ni}^{sb} V(J) \right] \quad (\text{II.27})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^b(J))^{N+1}} = -\delta_{il} \Delta t A(J) R_n(J) \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad (\text{II.28})$$

(3) For particulate chemicals on bed sediments:

$$\frac{\partial \text{RESC}_k}{\partial (C_1^w(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bf} M_n(J) \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad (\text{II.29})$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^s(J))^{N+1}} = -\delta_{il} \Delta t D_n(J) \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad (\text{II.30})$$

$$\frac{\partial \text{RESC}_k}{\partial (C_{nl}^b(J))^{N+1}} = \delta_{il} M_n(J) + \delta_{il} \Delta t R_n(J) + \delta_{il} \Delta t M_n(J) \left[\lambda_{ni}^b + k_{ni}^{bb} \right] \quad (\text{II.31})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

Subroutine JACOBI_2

This subroutine is to compute the Jacobian for the chemical system at the NP-th node. The Jacobian elements are defined as follows.

(1) For dissolved chemicals:

$$\frac{\partial \text{RES}(i)}{\partial (C_1^w)^{N+1}} = \delta_{il} h + \delta_{il} \delta t \left[\lambda_i^w h + R - I + h k_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} \right] - \delta t \left[\sum_{m=1}^{N_{rx}} k_m^{rb} h b_{mi} (C_1^w)^{b_{mi}-1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{b_{mj}} - \sum_{m=1}^{N_{rx}} k_m^{rf} h a_{mi} (C_1^w)^{a_{mi}-1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{a_{mj}} \right] \quad (II.32)$$

$i \in [1, N_c]$

$$\frac{\partial \text{RES}(i)}{\partial (C_{nl}^s)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sb} S_n h \quad n \in [1, N_s], \quad i \in [1, N_c], \quad (II.33)$$

$$\frac{\partial \text{RES}(i)}{\partial (C_{nl}^b)^{N+1}} = -\delta_{il} \delta t k_{ni}^{bb} M_n \quad n \in [1, N_s], \quad i \in [1, N_c] \quad (II.34)$$

(2) For particulate chemicals on suspended sediments:

$$\frac{\partial \text{RES}(k)}{\partial (C_1^w)^{N+1}} = -\delta_{il} \delta t k_{ni}^{sf} S_n h \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad (II.35)$$

$$\frac{\partial \text{RES}(k)}{\partial (C_{nl}^s)^{N+1}} = \delta_{il} h S_n + \delta_{il} \delta t D_n + \delta_{il} \delta t S_n \left[\lambda_i^s h + k_{ni}^{sb} h + R - I \right] \quad (II.36)$$

$n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i$

$$\frac{\partial \text{RES}(k)}{\partial (C_{nl}^b)^{N+1}} = -\delta_{il} \delta t R_n \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad (II.37)$$

(3) For particulate chemicals on bed sediments:

$$\frac{\partial \text{RES}(k)}{\partial (C_1^w)^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bf} M_n \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad (II.38)$$

$$\frac{\partial \text{RES}(k)}{\partial (C_{nl}^s)^{N+1}} = -\delta_{il} \Delta t D_n \quad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad (II.39)$$

$$\frac{\partial \text{RES}(k)}{\partial (C_{ni}^b)^{N+1}} = \delta_{il} M_n + \delta_{il} \Delta t R_n + \delta_{il} \Delta t M_n \left[\lambda_{ni}^b + k_{ni}^{bb} \right] \quad (\text{II.40})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

It is noted that if SS, and R are negative (i.e., sinks), they should not appear in Eqs. (II.32) and (II.36). Likewise, if I is positive (i.e., sink), it must not appear in the two equations.

Subroutine JACOBI_3

This subroutine is to compute the Jacobian for the chemical system at the NP-th node. The Jacobian elements are defined as follows.

(1) For dissolved chemicals:

$$\begin{aligned} \frac{\partial (\text{RES}_i^c)}{\partial (C_1^w)^{N+1}} &= \delta_{il} \theta + \delta_{il} \delta t \left(\lambda_i^c \theta + q \right) \\ &- \delta t \left[\sum_{m=1}^{N_{rx}} (a_{mi}^c - b_{mi}^c) \theta \left(k_m^{rb} b_{ml}^c (C_1^w)^{b_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{b_{mj}^c} - k_m^{rf} a_{ml}^c (C_1^w)^{a_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{a_{mj}^c} \right) \right. \\ &+ \sum_{m=1}^{N_{rxs}} (a_{mi}^c - b_{mi}^c) \theta \left(k_m^{sb} b_{ml}^c (C_1^w)^{b_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right. \\ &\left. \left. - k_m^{sf} a_{ml}^c (C_1^w)^{a_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} \right) \right] \quad i \in [1, N_c] \end{aligned} \quad (\text{II.41})$$

$$\frac{\partial (\text{RES}_i^c)}{\partial (S_l)^{N+1}} = \delta t \sum_{m=1}^{N_{rxs}} (a_{mi}^c - b_{mi}^c) \theta k_m^{sf} a_{ml}^c (S_l)^{a_{ml}^s - 1} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1, j \neq l}^{N_s} (S_j)^{a_{mj}^s} \quad i \in [1, N_c] \quad (\text{II.42})$$

$$\frac{\partial (\text{RES}_i^c)}{\partial (D_l)^{N+1}} = -\delta t \sum_{m=1}^{N_{rxs}} (a_{mi}^c - b_{mi}^c) \theta k_m^{sb} b_{ml}^c (D_l)^{b_{ml}^d - 1} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1, j \neq l}^{N_d} (D_j)^{b_{mj}^d} \quad i \in [1, N_c] \quad (\text{II.43})$$

(2) For adsorbing sites:

$$\begin{aligned} \frac{\partial (\text{RES}_i^s)}{\partial (C_1^w)^{N+1}} &= -\Delta t \sum_{m=1}^{N_{rxs}} a_{mi}^s \theta \left[k_m^{sb} b_{ml}^c (C_1^w)^{b_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right. \\ &\left. - k_m^{sf} a_{ml}^c (C_1^w)^{a_{ml}^c - 1} \prod_{j=1, j \neq l}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} \right] \quad i \in [1, N_s] \end{aligned} \quad (\text{II.44})$$

$$\frac{\partial(\text{RES}_i^s)}{\partial(S_i)^{N+1}} = \delta_{ii} \theta + \delta_{ii} \Delta t \theta \lambda_j^s$$

$$+ \Delta t \left[\sum_{m=1}^{N_{rs}} a_{mi}^s \theta k_m^{sf} a_{mi}^s (S_i)^{a_{mi}^s - 1} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1, j \neq i}^{N_s} (S_j)^{a_{mj}^s} \right] \quad i \in [1, N_s]$$
(II.45)

$$\frac{\partial(\text{RES}_i^s)}{\partial(D_i)^{N+1}} = -\Delta t \sum_{m=1}^{N_{rs}} a_{mi}^s \theta k_m^{sb} b_{mi}^d (D_i)^{b_{mi}^d - 1} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1, j \neq i}^{N_d} (D_j)^{b_{mj}^d} \quad i \in [1, N_s]$$
(II.46)

(3) For adsorbed chemicals:

$$\frac{\partial(\text{RES}_i^d)}{\partial(C_i^w)^{N+1}} = \Delta t \sum_{m=1}^{N_{rs}} b_{mi}^d \theta \left[k_m^{sb} b_{mi}^c (C_i^w)^{b_{mi}^c - 1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right.$$

$$\left. - k_m^{sf} a_{mi}^c (C_i^w)^{a_{mi}^c - 1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} \right] \quad i \in [1, N_d]$$
(II.47)

$$\frac{\partial(\text{RES}_i^d)}{\partial(S_i)^{N+1}} = -\Delta t \sum_{m=1}^{N_{rs}} b_{mi}^d \theta k_m^{sf} a_{mi}^s (S_i)^{a_{mi}^s - 1} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1, j \neq i}^{N_s} (S_j)^{a_{mj}^s} \quad i \in [1, N_d]$$
(II.48)

$$\frac{\partial(\text{RES}_i^d)}{\partial(D_i)^{N+1}} = \delta_{ii} \theta + \delta_{ii} \Delta t \theta \lambda_j^d$$

$$+ \Delta t \sum_{m=1}^{N_{rs}} b_{mi}^d \theta k_m^{sb} b_{mi}^d (D_i)^{b_{mi}^d - 1} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1, j \neq i}^{N_d} (D_j)^{b_{mj}^d} \quad i \in [1, N_d]$$
(II.49)

It is noted that if q is negative (i.e., sink), it should not appear in Eq. (II.41).

Subroutine JUNCTION

This subroutine is to update water depths (stages) at junctions based on the concept of water budget.

Subroutine KXKY_2M

This subroutine is to determine characteristic directions at a 2-D global node for overland flow simulations, based on the velocity, the spatial velocity derivatives, and the spatial stage derivatives at the node. This subroutine is needed only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine KXKYNP2M

This subroutine is to determine characteristic directions at all 2-D global nodes for overland flow simulations. This subroutine is needed only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine LINEAR

This subroutine is to determine a functional value through linear interpolation.

Subroutine LLTINV

This subroutine is to solve for a modified residual that is to be used in the preconditioned conjugate gradient algorithm.

Subroutine LNDGEN_2

This subroutine is to determine node-node and node-element connectivity in 2-D simulations, based on the given element indices.

Subroutine LOCPLN_3

This subroutine is to determine the interpolation functions for a node that is located on a 3-D element side, given the global coordinates of the node and the element side nodes.

Subroutine LOCQ_1

This subroutine is to locate the target point and its velocity for a tracking path in a 1-D subelement of particle tracking.

Subroutine LOCQ_2

This subroutine is to locate the target point and its velocity for a tracking path in a 2-D subelement of particle tracking. The available tracking time left after this tracking path is also computed.

Subroutine LOCQ2M

This subroutine is to locate the target point and its velocity for a tracking path in a 2-D subelement of particle tracking. The available tracking time left after this tracking path is also computed. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine LOCQ_32

This subroutine is to locate the target point and its velocity for a tracking path on a 3-D boundary side when the tracking along boundary is being considered. The available tracking time left after this tracking path is also computed.

Subroutine LOCQ_3

This subroutine is to locate the target point and its velocity for a tracking path in a 3-D subelement of particle tracking when the target side has been determined to be triangular. The available tracking time left after this tracking path is also computed.

Subroutine LOCQ_4

This subroutine is to locate the target point and its velocity for a tracking path in a 2-D subelement of particle tracking when the target side has been determined to be quadrilateral. The available tracking time left after this tracking path is also computed.

Subroutine LRL_3

This subroutine is to generate arrays describing 3-D node-element connectivity, given element indices.

Subroutine LRN_3

This subroutine is to generate arrays describing 3-D node-node connectivity, give element indices.

Subroutine MMLOC_2

This subroutine is to specify the starting location to start the 2-D "in-element" particle tracking in an element.

Subroutine MMLOC_3

This subroutine is to specify the starting location to start the 3-D "in-element" particle tracking in an element.

Subroutine NELIM

This subroutine is to prepare an array consisting of nodal numbers from a set of element face data.

Subroutine NEWXE

This subroutine is to determine the new iteration parameters for locating the target point in Subroutines LOCQ_3 and LOCQ_4.

Subroutine NODV_1

This subroutine is to calculate Manning's n at every 1-D global node.

Subroutine NODV_2

This subroutine is to calculate Manning's n at every 2-D global node.

Subroutine NUDZ0_1

This subroutine is to compute the source term, which is coming from non-uniform bed slopes (in the case of kinematic model) or stage slope (in the case of diffusive model), for all global nodes in 1-D river/stream flow simulations.

Subroutine NUDZ0_2

This subroutine is to compute the source term, which is coming from non-uniform bed slopes (in the case of kinematic model) or stage slope (in the case of diffusive model), for all global nodes in 2-D overland flow simulations.

Subroutine OBCOEF2M

This subroutine is to determine the coefficient of a characteristic at an open boundary node. The characteristic has been determined coming from the outside of the domain. This subroutine is needed only when the method of characteristics approach is taken to solve 2-D overland flow equations.

Subroutine ONLINE_2

This subroutine is to adjust the coordinates of a specified point if needed, such that this point will be located on the line segment with two given 2-D nodes serving as its end nodes.

Subroutine ONLINE_3

This subroutine is to adjust the coordinates of a specified point if needed, such that this point will be located on the line segment with two given 3-D nodes serving as its end nodes.

Subroutine ONPLAN_3

This subroutine is to adjust the coordinates of a specified point if needed, such that this point will

be located on the element side with three or four given nodes serving as the side nodes.

Subroutine PAGEN_1

This subroutine is to generate 1-D pointer arrays needed for numerical simulations.

Subroutine PAGEN_2

This subroutine is to generate 2-D pointer arrays needed for numerical simulations.

Subroutine PAGEN_3

This subroutine is to generate 3-D pointer arrays needed for numerical simulations.

Subroutine PFFCT1

This subroutine is to determine the functional value by interpolation from a given profile.

Subroutine PFFCT2

This subroutine is to determine the functional values of an array by interpolation from a series of given profiles.

Subroutine PWISS

This subroutine is to solve the linearized matrix equation with a pointwise iteration solution strategy.

Subroutine PLANEW_3

This subroutine is to determine which one of the two sides, separated by a specified plane, the particle would move onto.

Subroutine POLYP

This subroutine is to solve a modified residual that is to be used in the preconditioned conjugate gradient algorithm.

Subroutine PPCG

This subroutine is to solve the linearized matrix equation with the preconditioned conjugate gradient method by using a polynomial as a preconditioner.

Subroutine PREPAR2M

This subroutine is to prepare for data needed to construct and solve the set of algebraic equations in Subroutine ASOLV2M.

Subroutine PRINTT_1

This subroutine is to write out simulation results of 1-D river/stream simulations at desired times.

Subroutine PRINTT_2

This subroutine is to write out simulation results of 2-D overland simulations at desired times.

Subroutine PRINTT_3

This subroutine is to write out simulation results of 3-D subsurface simulations at desired times.

Subroutine Q2FLUX

This subroutine is to perform boundary integration over a 2-D boundary side.

Subroutine Q2F1

This subroutine is to determine element coefficient matrices and load vectors to compute the gradients of bottom elevation, water stage, velocities, and Manning's n in 1-D river/stream flow simulations.

Subroutine Q2F2

This subroutine is to determine element coefficient matrices and load vectors to compute the gradients of the derivatives of bottom elevation in 1-D river/stream flow simulations.

Subroutine Q2F3

This subroutine is to determine element coefficient matrices and load vectors to compute the gradients of hydraulic radius and average river/stream width in 1-D river/stream flow simulations.

Subroutine Q2T

This subroutine is to determine the line element coefficient matrices and load vectors to solve 1-D transport equation in the Eulerian step.

Subroutine Q3T

This subroutine is to determine the triangular element coefficient matrices and load vectors to solve 2-D transport equation in the Eulerian step.

Subroutine Q4T

This subroutine is to determine the quadrilateral element coefficient matrices and load vectors to solve 2-D transport equation in the Eulerian step.

Subroutine Q34ADBT

This subroutine is to implement flux-type boundary conditions, Cauchy or Variable, on a specified boundary side (quadrilateral or triangular) for the Lagrangian step in simulating 3-D subsurface dissolved chemical transport. The computed element load vectors are to be assembled in Subroutine ADVBCT_3 in order to determine the Lagrangian concentration on the boundary.

Subroutine Q34ADBT

This subroutine is to implement the surface/subsurface interface boundary condition on an interface boundary side (quadrilateral or triangular) for the Lagrangian step in simulating 3-D subsurface dissolved chemical transport. The computed element vectors are to be assembled in Subroutine ADVBCT_3 in order to determine the Lagrangian concentration on the boundary.

Subroutine Q34CNV

This subroutine is to implement flux-type boundary conditions, Cauchy, Neumann, or Variable, on a specified boundary side (quadrilateral or triangular) for the Eulerian step in simulating 3-D subsurface dissolved chemical transport. The computed element matrices and load vectors are to be assembled in Subroutine BCT_3 in order to determine the intermediate concentration (i.e., $(C_i^*)^{N+1/2}$) on the boundary.

Subroutine Q34CNV

This subroutine is to implement surface/subsurface interface boundary condition on an interface boundary side (quadrilateral or triangular) for the Eulerian step in simulating 3-D subsurface dissolved chemical transport. The computed element matrices and load vectors are to be assembled in Subroutine

BCT_3 in order to determine the intermediate concentration (i.e., $(C_i^w)^{N+1/2}$) on the boundary.

Subroutine Q34FM

This subroutine is to determine the element coefficient matrices, including mass matrices and the stiffness matrices taking into account eddy viscosity in solving 2-D dynamic wave model.

Subroutine Q34F1

This subroutine is to determine element coefficient matrices and load vectors to compute the gradients of bottom elevation, water stage, velocities, and Manning's n in 2-D overland flow simulations.

Subroutine Q34F2

This subroutine is to determine element coefficient matrices and load vectors to compute the gradients of the derivatives of bottom elevation in 2-D overland flow simulations.

Subroutine Q34R

This subroutine is to implement the river boundary condition on a specified boundary side in simulating 3-D subsurface flow. The computed element matrices and load vectors are assembled in Subroutine BCF_3 in order to compute the spatial distribution of pressure head at the time of interest.

Subroutine Q34S

This subroutine is to implement flux type boundary conditions, including Cauchy, Neumann, Variable, and surface/subsurface interface boundary conditions, on a specified boundary side in simulating 3-D subsurface flow. The computed element load vectors are assembled in Subroutine BCF_3 in order to compute the spatial distribution of pressure head at the time of interest.

Subroutine Q468DVF

This subroutine is to compute the element matrices and load vectors for calculating the Darcy velocity (specific discharge). The computed element matrices and load vectors are assembled in Subroutine VELT_3.

Subroutine Q468F

This subroutine is to compute the element matrices and load vectors for solving the 3-D subsurface flow equation. The computed element matrices and load vectors are assembled in Subroutine ASEMBF_3.

Subroutine Q468T

This subroutine is to compute the element matrices and load vectors for solving the 3-D subsurface transport equation of dissolved chemicals in the predictor step. The computed element matrices and load vectors are assembled in Subroutine ASEMBT_3.

Subroutine Q468TH

This subroutine is to compute the element load vectors for computing the contribution of the increasing rate of the moisture content.

Subroutine RAINOD_1

This subroutine is to determine rainfall rate at 1-D global nodes.

Subroutine RAINOD_2

This subroutine is to determine rainfall rate at 2-D global nodes.

Subroutine REPLAS_2

This subroutine is to write the values of the first four arguments into the last four arguments.

Subroutine REPLAS_3

This subroutine is to write the values of the first six arguments into the last six arguments.

Subroutine RESIDU_1

This subroutine is to compute the residual of the 1-D transport equations of (1) dissolved chemicals (when ID = 1), (2) particulate chemicals on suspended sediments (when ID = 1), (3) particulate chemicals on bed sediments (when ID = 1), and (4) suspended sediments (when ID = 2) at the NP-th node (when NP is not equal to zero and J equals zero) or the J-th junction (when NP equals zero and J is not equal to zero). The residuals are defined as follows.

For the case at the NP-th node:

(1) For dissolved chemicals:

$$RESC_i = A \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t (RHSC_i)^{N+1} + \delta t (RHSC_i)^N \quad i \in [1, N_c] \quad (II.50)$$

(2) For particulate chemicals on suspended sediments:

$$RESC_k = A \left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2} \right] - \delta t (RHSC_k)^{N+1} + \delta t (RHSC_k)^N \quad (II.51)$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i$$

(3) For particulate chemicals on bed sediments:

$$RESC_k = (M_n C_{ni}^b)^{N+1} - (M_n C_{ni}^b)^N - \Delta t (RHSC_k)^{N+1} \quad (II.52)$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

(4) For suspended sediments:

$$RESS_n = A (S_n)^{N+1/2} + \delta t (RHSS_n)^{N+1} - \delta t (RHSS_n)^N \quad n \in [1, N_s] \quad (II.53)$$

where $(RHSS_n)^{N+1}$ is evaluated with ID = 22 in Subroutine RHSCOMP1, whereas $(RHSS_n)^N$ is calculated with ID = 21.

For the case at the J-th junction:

(1) For dissolved chemicals:

$$RESC_i = \left[(V(J) C_i^w(J))^{N+1} - (V(J) C_i^w(J))^N \right] - \Delta t (RHSC_i)^{N+1} \quad i \in [1, N_c] \quad (II.54)$$

(2) For particulate chemicals on suspended sediments:

$$RESC_k = \left[(V(J) S_n(J) C_{ni}^s(J))^{N+1} - (V(J) S_n(J) C_{ni}^s(J))^N \right] - \Delta t (RHSC_k)^{N+1} \quad (II.55)$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i$$

(3) For particulate chemicals on bed sediments:

$$\text{RESC}_k = (M_n(J)C_{ni}^b(J))^{N+1} - (M_n(J)C_{ni}^b(J))^N - \Delta t (\text{RHSC}_k)^{N+1} \quad (\text{II.56})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

(4) For suspended sediments:

$$\text{RESS}_n = (V(J)S_n(J))^N + \Delta t (\text{RHSS}_n)^{N+1} \quad n \in [1, N_s] \quad (\text{II.57})$$

Subroutine RESIDU_2

This subroutine is to compute the residual of the 2-D transport equations of (1) dissolved chemicals (when ID = 1), (2) particulate chemicals on suspended sediments (when ID = 1), (3) particulate chemicals on bed sediments (when ID = 1), and (4) suspended sediments (when ID = 2) at the NP-th node. The residuals are defined as follows.

(1) For dissolved chemicals:

$$\text{RESC}_i = h \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t (\text{RHSC}_i)^{N+1} + \delta t (\text{RHSC}_i)^N \quad i \in [1, N_c] \quad (\text{II.58})$$

(2) For particulate chemicals on suspended sediments:

$$\text{RESC}_k = h \left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2} \right] - \delta t (\text{RHSC}_k)^{N+1} + \delta t (\text{RHSC}_k)^N \quad (\text{II.59})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i$$

(3) For particulate chemicals on bed sediments:

$$\text{RESC}_k = (M_n C_{ni}^b)^{N+1} - (M_n C_{ni}^b)^N - \Delta t (\text{RHSC}_k)^{N+1} \quad (\text{II.60})$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

(4) For suspended sediments:

$$\text{RESS}_n = h(S_n)^{N+1/2} + \delta t (\text{RHSS}_n)^{N+1} - \delta t (\text{RHSS}_n)^N \quad n \in [1, N_s] \quad (\text{II.61})$$

where $(\text{RHSS}_n)^{N+1}$ is evaluated with ID = 22 in Subroutine RHSCOMP1, whereas $(\text{RHSS}_n)^N$ is calculated with ID = 21.

Subroutine RESIDU_3

This subroutine is to compute the residual of the 3-D transport equations of (1) dissolved chemicals, (2) adsorbing sites, and (3) adsorbed chemicals.

(1) For dissolved chemicals:

$$\begin{aligned} & (\text{RES}_i^c) \\ &= \theta \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t \left[(\text{RHS}_i^c)^{N+1} - (\text{RHS}_i^c)^N \right] \quad \left(\text{if } (\text{RHS}_i^c)^N \geq 0 \right) \\ &= \theta \left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2} \right] - \delta t \left[(\text{RHS}_i^c)^{N+1} - \frac{(\text{RHS}_i^c)^N}{(C_i^w)^N} (C_i^w)^{N+1/2} \right] \quad \left(\text{if } (\text{RHS}_i^c)^N < 0 \right) \quad i \in [1, N] \end{aligned} \quad (\text{II.62})$$

(2) For adsorbing sites:

$$(RES_j^s) = (\theta S_j)^{N+1} - (\theta S_j)^N - \Delta t (RHS_j^s)^{N+1} \quad j \in [1, N_s] \quad (II.63)$$

(3) For adsorbed chemicals:

$$(RES_j^d) = (\theta D_j)^{N+1} - (\theta D_j)^N - \Delta t (RHS_j^d)^{N+1} \quad j \in [1, N_d] \quad (II.64)$$

Subroutine RHSCMP_1

This subroutine is to compute the right-hand side of the 1-D transport governing equations of (1) dissolved chemicals (when ID = 1), (2) particulate chemicals on suspended sediments (when ID = 1), (3) particulate chemicals on bed sediments (when ID = 1), and (4) suspended sediments (when ID = 21 or 22) at the NP-th node (when NP is not equal to zero and J equals zero) or the J-th junction (when NP equals zero and J is not equal to zero). The right-hand sides are defined as follows.

For the case at the NP-th node:

(1) For dissolved chemicals:

$$\begin{aligned} RHSC_i = & \left[M_i^{cw} + A k_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n A C_{ni}^s + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n P C_{ni}^b + \sum_{m=1}^{N_{rx}} k_m^{rb} A \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}} + M_i^{crw} - M_i^{ciw} + M_i^{cow} \right] \\ & - \left[\lambda_i^w A + A k_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} + \sum_{m=1}^{N_{rx}} k_m^{rf} A (C_i^w)^{a_{mi}-1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{a_{mj}} + R - I + R_1 + R_2 \right] C_i^w \\ & i \in [1, N_c] \end{aligned} \quad (II.65)$$

(2) For particulate chemicals on suspended sediments:

$$\begin{aligned} RHSC_k = & \left[M_{ni}^{cs} + k_{ni}^{sf} S_n A C_i^w + B R_n C_{ni}^b - B D_n C_{ni}^s + M_{ni}^{cos} \right] \\ & - \left[\lambda_{ni}^s A + k_{ni}^{sb} A + R - I + R_1 + R_2 \right] S_n C_{ni}^s \quad n \in [1, N_s], i \in [1, N_c], k = n * N_c + i \end{aligned} \quad (II.66)$$

(3) For particulate chemicals on bed sediments:

$$\begin{aligned} RHSC_k = & \left[D_n C_{ni}^s - R_n C_{ni}^b + k_{ni}^{bf} M_n C_i^w \right] - \left[\lambda_{ni}^b + k_{ni}^{bb} \right] M_n C_{ni}^b \\ & n \in [1, N_s], i \in [1, N_c], k = (n + N_s) * N_c + i \end{aligned} \quad (II.67)$$

(4) For suspended sediments:

(a) when ID = 21,

$$RHSS_n = \left[M_n^s + P R_n - P D_n + M_n^{os} \right] - \left[R - I + R_1 + R_2 \right] S_n \quad n \in [1, N_s] \quad (II.68)$$

(b) when ID = 22,

$$RHSS_n = [M_n^s + PR_n - PD_n + M_n^{os}] \quad n \in [1, N_s] \quad (II.69)$$

For the case at the J-th junction:

(1) For dissolved chemicals:

$$\begin{aligned} RHSC_i = & \sum_{k=1}^{NJRTH(J)} Q^k C_i^{wk} + M_i^{cw}(J) - \lambda_i^w V(J) C_i^w(J) + M_i^{crw}(J) - M_i^{ciw}(J) + M_i^{cow}(J) + V(J) k_i^{ab} \left[p_i - \frac{k_i^{af}}{k_i^{ab}} C_i^w(J) \right] \\ & + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n(J) V(J) \left[C_{ni}^s(J) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w(J) \right] + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n(J) AJT(J) \left[C_{ni}^b(J) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w(J) \right] \\ & + \sum_{m=1}^{N_n} k_m^{rb} V(J) \left[\prod_{j=1}^{N_c} (C_j^w(J))^{b_{mj}} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w(J))^{a_{mj}} \right] \quad i \in [1, N_c] \end{aligned} \quad (II.70)$$

(2) For particulate chemicals on suspended sediments:

$$\begin{aligned} RHSC_k = & \sum_{k=1}^{NJRTH(j)} Q^k S_n C_{ni}^{sk} + M_{ni}^{cs}(J) - \lambda_{ni}^s V(J) S_n(J) C_{ni}^s(J) - k_{ni}^{sb} S_n(J) V(J) \left[C_{ni}^s(J) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w(J) \right] \\ & + R_n(J) AJT(J) C_{ni}^b(J) - D_n(J) AJT(J) C_{ni}^s(J) + M_{ni}^{cos}(J) \quad n \in [1, N_s], i \in [1, N_c], k = n * N_c + i \end{aligned} \quad (II.71)$$

(3) For particulate chemicals on bed sediments:

$$\begin{aligned} RHSC_k = & [D_n(J) C_{ni}^s(J) - R_n(J) C_{ni}^b(J)] - \lambda_{ni}^b M_n(J) C_{ni}^b(J) - k_{ni}^{bb} M_n(J) \left[C_{ni}^b(J) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w(J) \right] \\ & n \in [1, N_s], i \in [1, N_c], k = (n + N_s) * N_c + i \end{aligned} \quad (II.72)$$

(4) For suspended sediments:

$$RHSS_n = \sum_{k=1}^{NJRTH(j)} Q^k S_n^k + M_n^s(J) + M_n^{os}(J) + [R_n(J) - D_n(J)] AJT(J) \quad n \in [1, N_s] \quad (II.73)$$

Subroutine RHSCMP_2

This subroutine is to compute the right-hand side of the 2-D transport governing equations of (1) dissolved chemicals (when ID = 1), (2) particulate chemicals on suspended sediments (when ID = 1), (3) particulate chemicals on bed sediments (when ID = 1), and (4) suspended sediments (when ID = 21 or 22) at the NP-th node. The right-hand sides are defined as follows.

(1) For dissolved chemicals:

$$\begin{aligned} \text{RHSC}_i = & \left[M_i^{cw} + h k_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n h C_{ni}^s + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n C_{ni}^b + \sum_{m=1}^{N_{rx}} k_m^{rb} h \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}} + M_i^{crw} - M_i^{ciw} \right] \\ & - \left[\lambda_i^w h + h k_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} + \sum_{m=1}^{N_{rx}} k_m^{rf} h (C_i^w)^{a_{mi}-1} \prod_{j=1, j \neq i}^{N_c} (C_j^w)^{a_{mj}} + R - I \right] C_i^w \quad i \in [1, N_c] \end{aligned} \quad (\text{II.74})$$

(2) For particulate chemicals on suspended sediments:

$$\begin{aligned} \text{RHSC}_k = & \left[M_{ni}^{cs} + k_{ni}^{sf} h S_n C_i^w + R_n C_{ni}^b - D_n C_{ni}^s \right] - \left[\lambda_{ni}^s h + k_{ni}^{sb} h + R - I \right] S_n C_{ni}^s \\ & n \in [1, N_s], i \in [1, N_c], k = n * N_c + i \end{aligned} \quad (\text{II.75})$$

(3) For particulate chemicals on bed sediments:

$$\begin{aligned} \text{RHSC}_k = & \left[D_n C_{ni}^s - R_n C_{ni}^b + k_{ni}^{bf} M_n C_i^w \right] - \left[\lambda_{ni}^b + k_{ni}^{bb} \right] M_n C_{ni}^b \\ & n \in [1, N_s], i \in [1, N_c], k = (n + N_s) * N_c + i \end{aligned} \quad (\text{II.76})$$

(4) For suspended sediments:

(a) when ID = 21,

$$\text{RHSS}_n = \left[M_n^s + R_n - D_n \right] - [R - I] S_n \quad n \in [1, N_s] \quad (\text{II.77})$$

(a) when ID = 22,

$$\text{RHSS}_n = \left[M_n^s + R_n - D_n \right] \quad n \in [1, N_s] \quad (\text{II.78})$$

Subroutine RHSCMP_3

This subroutine is compute the right hand side of the 3-D transport equations of (1) dissolved chemicals, (2) adsorbing sites, and (3) adsorbed chemicals.

(1) For dissolved chemicals:

$$\begin{aligned} \text{RHS}_i^c = & q \left[C_j^{\text{in}} - C_j^w \right] - \lambda_j^c \theta C_j^w - \sum_{m=1}^{N_{rx}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{rf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} - k_m^{rb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \right] \\ & - \sum_{m=1}^{N_{rxs}} (a_{mj}^c - b_{mj}^c) \theta \left[k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_c] \end{aligned} \quad (\text{II.79})$$

(2) For adsorbing sites:

$$\begin{aligned} \text{RHS}_j^s &= -\lambda_j^s \theta S_j - \sum_{m=1}^{N_{rs}} a_{mj}^s \theta \left[k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_s] \end{aligned} \quad (\text{II.80})$$

(3) For adsorbed chemicals:

$$\begin{aligned} \text{RHS}_j^d &= -\lambda_j^d \theta D_j + \sum_{m=1}^{N_{rs}} b_{mj}^d \theta \left[k_m^{sf} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}^c} \prod_{j=1}^{N_s} (S_j)^{a_{mj}^s} - k_m^{sb} \prod_{j=1}^{N_c} (C_j^w)^{b_{mj}^c} \prod_{j=1}^{N_d} (D_j)^{b_{mj}^d} \right] \quad j \in [1, N_d] \end{aligned} \quad (\text{II.81})$$

Subroutine RINCS

This subroutine is to read in chemistry and sediment information.

Subroutine RINF_1

This subroutine is to read in information for 1-D river/stream flow simulations.

Subroutine RINF_2

This subroutine is to read in information for 2-D overland flow simulations.

Subroutine RINF_3

This subroutine is to read in information for 3-D subsurface flow simulations.

Subroutine RINIT_1

This subroutine is to read in the initial condition for 1-D river/stream flow and/or transport simulations.

Subroutine RINIT_2

This subroutine is to read in the initial condition for 2-D overland flow and/or transport simulations.

Subroutine RINIT_3

This subroutine is to read in the initial condition for 3-D subsurface flow and/or transport simulations.

Subroutine RINT_1

This subroutine is to read in information for 1-D river/stream transport.

Subroutine RINT_2

This subroutine is to read in information for 2-D overland transport.

Subroutine RINT_3

This subroutine is to read in information for 3-D subsurface transport.

Subroutine SFLOWF_3

This subroutine is to compute flow fluxes through various types of boundary and the increasing rate

of moisture content in the domain of interest. The detailed description for this subroutine can be found elsewhere [Yeh et al, 1997].

Subroutine SHAPE_3

This subroutine is to compute shape functions and their derivatives, given the local coordinates, natural coordinates, or Cartesian coordinates of the node of interest and its associated element nodes.

Subroutine SOL_BS

This subroutine is to solve the transport governing equation of bed sediments at the NP-th river/stream or overland node.

Subroutine SOL_BSJT

This subroutine is to solve the transport governing equation of bed sediments at the IJT-th junction..

Subroutine SOL_C1

This subroutine is to solve for the concentrations of dissolved chemicals, particulate chemicals on suspended sediments, and particulate sediments on bed sediments at 1-D global nodes (when ID = 1) or at junctions (when ID = 2). For the case at global nodes, this subroutine serves as the corrector step in our predictor-corrector approach to solve transport equations of chemicals. For the case at junctions, the governing equations accounting for chemical interactions are solved in this subroutine. The Newton-Raphson method is employed to solve the nonlinear system of chemical reactions. The full-pivoting technique is incorporated into a direct solver to handle linearized matrix equations.

Subroutine SOL_C2

This subroutine is to solve for the concentrations of dissolved chemicals, particulate chemicals on suspended sediments, and particulate sediments on bed sediments at 2-D global nodes. This subroutine serves as the corrector step in our predictor-corrector approach to solve transport equations of chemicals. The Newton-Raphson method is employed to solve the nonlinear system of chemical reactions. The full-pivoting technique is incorporated into a direct solver to handle linearized matrix equations.

Subroutine SOL_C3

This subroutine is to solve for the concentrations of dissolved chemicals, adsorbing sites, and adsorbed chemicals at 3-D global nodes. This subroutine serves as the corrector step in our predictor-corrector approach to solve transport equations of chemicals. The Newton-Raphson method is employed to solve the nonlinear system of chemical reactions. The full-pivoting technique is incorporated into a direct solver to handle linearized matrix equations.

Subroutine SOL_SS1

This subroutine is to solve the concentrations of suspended sediments at the NP-th river/stream node in the corrector step, where the time-implicit scheme is employed.

Subroutine SOL_SS2

This subroutine is to solve the concentrations of suspended sediments at the NP-th overland node in the corrector step, where the time-implicit scheme is employed.

Subroutine SOL_SSJT

This subroutine is to solve the concentrations of suspended sediments at the IJT-th junction, where the time-implicit scheme is employed.

Subroutine SORT

This subroutine is to compress the material ID so that there is no skip number in the material IDs and the material ID is expected to increase sequentially from 1 to the number of materials.

Subroutine SPROP_3

This subroutine is to compute moisture content, water capacity, and hydraulic conductivity in all subsurface elements.

Subroutine STAR2M

This subroutine is to determine the Lagrangian values (i.e., H_1^* , u_1^* , v_1^* , H_2^* , u_2^* , v_2^* , H_3^* , u_3^* , v_3^* appeared in Section 3.2.1) associated with each characteristic.

Subroutine STORE_1D

This subroutine is to store the computer results of 1-D river/stream in a binary file for further plotting purposes.

Subroutine STORE_2D

This subroutine is to store the computer results of 2-D overland in a binary file for further plotting purposes.

Subroutine STORE_3D

This subroutine is to store the computer results of 3-D subsurface in a binary file for further plotting purposes.

Subroutine STRIP

This subroutine is to read in a character variable.

Subroutine SURE_2

This subroutine is to analytically determine the target location of a 2-D tracking path when the single-velocity approach is applied.

Subroutine SURE2M

This subroutine is to analytically determine the target location of a 2-D tracking path when the single-velocity approach is applied. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine SUR2D3

This subroutine is to analytically determine the target location of a 2-D tracking path on a 3-D boundary side when the single-velocity approach is applied.

Subroutine SURE_3

This subroutine is to analytically determine the target location of a 3-D tracking path when the single-velocity approach is applied.

Subroutine SURF_2

This subroutine is to generate boundary arrays for implementing boundary conditions in 2-D simulations.

Subroutine SURF_3

This subroutine is to generate boundary arrays for implementing boundary conditions in 3-D simulations.

Subroutine THNODE_3

This subroutine is to compute moisture content at all subsurface nodes.

Subroutine TRAK_V1

This subroutine is to determine the tracking velocity for implementation of the Lagrangian step of 1-D river/stream flow computation

Subroutine TRAK_1

This subroutine is to determine the target location of a tracking path in a 1-D subelement.

Subroutine TRAK_21

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is where an subelement node is located.

Subroutine TRAK_22

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is not where an subelement node is located.

Subroutine TRAK21M

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is where an subelement node is located. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine TRAK22M

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is not where an subelement node is located. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine TRAK_31H

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working hexahedral subelement. This subroutine is employed when the starting location is where an subelement node is located.

Subroutine TRAK_31P

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the

working triangular prism subelement. This subroutine is employed when the starting location is where an subelement node is located.

Subroutine TRAK_31T

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working tetrahedral subelement. This subroutine is employed when the starting location is where an subelement node is located.

Subroutine TRAK_32H

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working hexahedral subelement. This subroutine is employed when the starting location is not where an subelement node is located.

Subroutine TRAK_32P

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working triangular prism subelement. This subroutine is employed when the starting location is not where an subelement node is located.

Subroutine TRAK_32T

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working tetrahedral subelement. This subroutine is employed when the starting location is not where an subelement node is located.

Subroutine TRANSP_1

This subroutine serves as the control panel to compute both chemical and sediment transport of 1-D river/stream. The predictor-corrector numerical approach is employed to solve the transport equations of mobile materials, such as dissolved chemicals, suspended sediments, and particulate chemicals on suspended sediments. During each time step, The predictor step is first implemented to obtain the intermediate values for mobile materials. Sediment equations are then solved by using the Picard to handle their nonlinearity. The concentrations of chemicals are the last to solve for. The set of nonlinear ordinary differential equations is solved with the Newton-Raphson method node by node in the corrector step.

Subroutine TRANSP_2

This subroutine serves as the control panel to compute both chemical and sediment transport of 2-D overland. The predictor-corrector numerical approach is employed to solve the transport equations of mobile materials, such as dissolved chemicals, suspended sediments, and particulate chemicals on suspended sediments. During each time step, The predictor step is first implemented to obtain the intermediate values for mobile materials. Sediment equations are then solved by using the Picard to handle their nonlinearity. The concentrations of chemicals are the last to solve for. The set of nonlinear ordinary differential equations is solved with the Newton-Raphson method node by node in the corrector step.

Subroutine TRANSP_3

This subroutine serves as the control panel to compute chemical transport of 3-D subsurface. The predictor-corrector numerical approach is employed to solve the transport equations of mobile materials, such

as dissolved chemicals. During each time step, The predictor step is first implemented to obtain the intermediate values for mobile materials. The set of nonlinear ordinary differential equations that is accounting for the reaction rates of dissolved chemicals, adsorbing sites, and adsorbed chemicals is solved with the Newton-Raphson method node by node in the corrector step.

Subroutine TRILRN2M

This subroutine is to generate pointer arrays for the use in constructing the matrix equation for adjusting 2-D flow velocity in the last part of the method of characteristic approach.

Subroutine TSCONV

This subroutine is to retrieve desired profiles from given x-y series curves.

Subroutine TSCONVV

This subroutine is to retrieve desired profiles from given x-y series curves.

Subroutine TSCONV2

This subroutine is to retrieve desired profiles from given x-y series curves.

Subroutine VALBDL_2

This subroutine is to compute the velocity at a specified 2-D node by interpolation.

Subroutine VALBDL2M

This subroutine is to compute the velocity at a specified 2-D node by interpolation. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine VELT_1

This subroutine is to compute the kinematic or diffusion velocities at all river/stream nodes.

Subroutine VELT_2

This subroutine is to compute the kinematic or diffusion velocities at all overland nodes.

Subroutine VELT_3

This subroutine is to compute the Darcy velocity (specific discharge) at all subsurface nodes. The mass-lumping technique is employed.

Subroutine VOLUME

This subroutine is to compute the volume of a 3-D element, given the coordinates of element nodes and element indices.

Subroutine WRKARY_2

This subroutine is to prepare working arrays for particle tracking in either a 2-D element or a 2-D subelement.

Subroutine WRKARY2M

This subroutine is to prepare working arrays for particle tracking in either a 2-D element or a 2-D subelement. It is employed only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine WRKARY_3

This subroutine is to prepare working arrays for particle tracking in either a 3-D element or a 3-D subelement.

Subroutine XSI_2

This subroutine is to determine the local coordinates of a specified node that is located in a 2-D quadrilateral element, given the original Cartesian coordinates of both the node and element nodes.

Subroutine XSI_3

This subroutine is to determine the local coordinates of a specified node that is located in a 3-D hexahedral element, given the original Cartesian coordinates of both the node and element nodes.

Subroutine XSI_3P

This subroutine is to determine the local/natural coordinates of a specified node that is located in a 3-D triangular prism element, given the original Cartesian coordinates of both the node and element nodes.

Appendix III. PARAMETERS FOR RUNNING THE COMPUTER CODE

The following is the content of the including file, **wms123.inc**, which is required to compile and run the computer code of the model. One needs to modify **wms123.inc** in order to provide appropriate values for the code parameters as defined as follows.

```
C
C — CONTROL INTEGERS FOR THE SPATIAL DOMAIN OF 2-D OVERLAND FLOW
C
C MAXNPK2 : MAX. NO. OF NODES
C MAXELK2 : MAX. NO. OF ELEMENTS
C MXBNPK2 : MAX. NO. OF BOUNDARY NODAL POINTS
C MXBESK2 : MAX. NO. OF BOUNDARY ELEMENT SIDES
C MXJBDK2 : MAX. NO. OF GLOBAL NODES NEEDED TO DESCRIBE THE NODE-NODE CONNECTIVITY
C MXKBDK2 : MAX. NO. OF GLOBAL ELEMENT NEEDED TO DESCRIBE NODE-ELEMENT CONNECTIVITY
C
C   PARAMETER (MAXNPK2=275,MAXELK2=462,MXBNPK2=1000,MXBESK2=1000)
C   PARAMETER (MXJBDK2=20,MXKBDK2=20)
C
C — CONTROL INTEGERS FOR THE TIME DOMAIN OF 2-D OVERLAND FLOW
C
C MXNTIK2 : MAX. NO. OF TIME STEPS
C MXDTCK2 : MAX. NO. OF DELT CHANGES
C
C   PARAMETER (MXNTIK2=50000,MXDTCK2=20)
C
C — CONTROL INTEGERS FOR MATERIAL PROPERTIES OF 2-D OVERLAND FLOW
C
C MXMATK2 : MAX. NO. OF MATERIAL TYPES
C MXMPMK2 : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL
C
C   PARAMETER (MXMATK2=10,MXMPMK2=6)
C
C — CONTROL INTEGERS FOR RAINFALL OF 2-D OVERLAND FLOW
C
C MXRESK2 : MAX. NO. OF ELEMENTS WITH RAINFALL CONDITION
C MXRPRK2 : MAX. NO. OF RAINFALL PROFILES
C MXRDPK2 : MAX. NO. OF DATA POINTS ON THE RAINFALL PROFILE
C
C   PARAMETER (MXRESK2=MAXELK2,MXRPRK2=5,MXRDPK2=200)
C
C — CONTROL INTEGERS FOR SOURCE/SINK OF 2-D OVERLAND FLOW
C
C MXSPRK2 : MAX. NO. OF SOURCE/SINK PROFILES
C MXSDPK2 : MAX. NO. OF DATA POINTS ON THE SOURCE/SINK PROFILE
C
C   PARAMETER (MXSPRK2=5,MXSDPK2=200)
C
C — CONTROL INTEGERS FOR OPEN BOUNDARY CONDITIONS OF 2-D OVERLAND FLOW
C
C MXDNPK2 : MAX. NO. OF DIRICHLET BOUNDARY NODAL POINTS
C MXDPRK2 : MAX. NO. OF DIRICHLET BOUNDARY PROFILES
C MXDDPK2 : MAX. NO. OF DATA POINTS IN A DIRICHLET PROFILES
C MXCESK2 : MAX. NO. OF FLUX-TYPE BOUNDARY SIDES
C MXFPRK2 : MAX. NO. OF UPSTREAM BOUNDARY FLUX PROFILES
C MXFDPK2 : MAX. NO. OF DATA POINTS IN A UPSTREAM BOUNDARY PROFILE
C MXCPRK2 : MAX. NO. OF DEPTH- OR STAGE-DEPENDENT FLUX PROFILES
C MXCDPK2 : MAX. NO. OF DATA POINTS IN A DEPTH- OR STAGE-DEPENDENT FLUX PROFILE
C
C   PARAMETER (MXDNPK2=500,MXDPRK2=10,MXDDPK2=500)
C   PARAMETER (MXCESK2=500,MXFPRK2=10,MXFDPK2=300)
C   PARAMETER (MXCPRK2=3,MXCDPK2=300)
C
```


C — CONTROL INTEGERS FOR IMPERMEABLE BOUNDARY CONDITIONS OF 2-D OVERLAND FLOW
 C
 C MXIBPK2 : MAX. NO. OF IMPERMEABLE BOUNDARY NODAL POINTS
 C
 C PARAMETER (MXIBPK2=500)
 C
 C — CONTROL INTEGERS FOR SUB-ELEMENT TRACKING OF 2-D OVERLAND FLOW
 C
 C MXNPWK2 : MAX. NO. OF NODES FOR A SUB-ELEMENT TRACKING
 C MXELWK2 : MAX. NO. OF SUB-ELEMENTS FOR A SUB-ELEMENT TRACKING
 C
 C PARAMETER (MXNPWK2=121,MXELWK2=100)
 C
 C — CONTROL INTEGERS FOR HYDROGRAPH OF 2-D OVERLAND FLOW
 C
 C MXPNTK2 : MAX. NO. OF NODAL POINTS FOR THE LINE CROSS SECTION
 C MXLINK2 : MAX. NO. OF LINE CROSS SECTION CAN BE SELECTED
 C MXITPK2 : MAX. NO. OF DATA POINTS ON THE HYDROGRAPH
 C
 C PARAMETER (MXPNTK2=50,MXLINK2=10,MXITPK2=100)
 C
 C — CONTROL INTEGERS FOR 2-D OVERLAND TRANSPORT
 C
 C MXMMMK2 : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL FOR TRANSPORT
 C MXSRPK2 : MAX. NO. OF SOURCE/SINK PROFILES
 C MXSRDPK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A SOURCE/SINK PROFILE
 C MXCESTK2 : MAX. NO. OF FLUX-TYPE BOUNDARY SIDES OF TRANSPORT
 C MXCPRTK2 : MAX. NO. OF FLUX-TYPE BOUNDARY CONDITION PROFILES OF TRANSPORT
 C MXCDPTK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A FLUX-TYPE BOUNDARY
 C CONDITION PROFILE OF TRANSPORT
 C MXDNPTK2 : MAX. NO. OF DIRICHLET BOUNDARY NODES OF TRANSPORT
 C MXDPRTK2 : MAX. NO. OF DIRICHLET BOUNDARY CONDITION PROFILES OF TRANSPORT
 C MXDDPTK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A DIRICHLET BOUNDARY
 C CONDITION PROFILE OF TRANSPORT
 C MXRCPRK2 : MAX. NO. OF CHEMICAL CONCENTRATION PROFILES IN RAINFALL
 C MXRCDPK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A CHEMICAL CONCENTRATION
 C PROFILES IN RAINFALL
 C
 C PARAMETER (MXMMMK2=3)
 C PARAMETER (MXSRPK2=20,MXSRDPK2=20)
 C PARAMETER (MXRCPRK2=20,MXRCDPK2=20)
 C PARAMETER (MXDNPTK2=200,MXDPRTK2=200,MXDDPTK2=100)
 C PARAMETER (MXCESTK2=200,MXCPRTK2=200,MXCDPTK2=100)
 C
 C — CONTROL INTEGERS FOR THE SPATIAL DOMAIN OF 1-D CHANNEL FLOW
 C
 C MAXNPK1 : MAX. NO. OF NODES
 C MAXELK1 : MAX. NO. OF ELEMENTS
 C
 C PARAMETER (MAXNPK1=500,MAXELK1=500)
 C
 C — CONTROL INTEGERS FOR THE TIME DOMAIN OF 1-D CHANNEL FLOW
 C
 C MXNTIK1 : MAX. NO. OF TIME STEPS
 C MXDTCK1 : MAX. NO. OF DELT CHANGES
 C
 C PARAMETER (MXNTIK1=5000,MXDTCK1=20)
 C
 C — CONTROL INTEGERS FOR MATERIAL PROPERTIES OF 1-D CHANNEL FLOW
 C
 C MXMATK1 : MAX. NO. OF MATERIAL TYPES
 C MXMPMK1 : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL
 C
 C PARAMETER (MXMATK1=10,MXMPMK1=6)
 C

C --- CONTROL INTEGERS FOR RAINFALL OF 1-D CHANNEL FLOW
 C
 C MXRESK1 : MAX. NO. OF ELEMENTS WITH RAINFALL CONDITION
 C MXRPRK1 : MAX. NO. OF RAINFALL PROFILES
 C MXRDPK1 : MAX. NO. OF DATA POINTS ON THE RAINFALL PROFILE
 C
 C PARAMETER (MXRESK1=MAXELK1,MXRPRK1=5,MXRDPK1=200)
 C
 C --- CONTROL INTEGERS FOR SOURCE/SINK OF 1-D CHANNEL FLOW
 C
 C MXSPRK1 : MAX. NO. OF SOURCE/SINK PROFILES
 C MXSDPK1 : MAX. NO. OF DATA POINTS ON THE SOURCE/SINK PROFILE
 C MXSJPRK1 : MAX. NO. OF SOURCE/SINK PROFILES AT JUNCTIONS
 C MXSJDPK1 : MAX. NO. OF DATA POINTS ON THE SOURCE/SINK PROFILE
 C AT JUNCTIONS
 C
 C PARAMETER (MXSPRK1=5,MXSDPK1=200)
 C PARAMETER (MXSJPRK1=5,MXSJDPK1=200)
 C
 C --- CONTROL INTEGERS FOR OPEN BOUNDARY CONDITIONS OF 1-D CHANNEL
 C FLOW
 C
 C MXDNPK1 : MAX. NO. OF OPEN BOUNDARY NODAL POINTS
 C MXDPRK1 : MAX. NO. OF OPEN BOUNDARY PROFILES
 C MXDDPK1 : MAX. NO. OF DATA POINTS ON THE PROFILES
 C
 C PARAMETER (MXDNPK1=500,MXDPRK1=50,MXDDPK1=300)
 C PARAMETER (MXCPRK1=10,MXCDPK1=300)
 C
 C --- CONTROL INTEGERS FOR 1-D CHANNEL REACH NUMBER
 C
 C MXRHK1 : MAX. NO. OF CHANNEL REACH NUMBER
 C MXRHNP1 : MAX. NO. OF NODES INCLUDED IN A CHANNEL REACH
 C
 C PARAMETER (MXRHK1=10,MXRHNPK1=100)
 C
 C --- CONTROL INTEGERS FOR CROSS-SECTIONAL GEOMETRY FOR 1-D CHANNEL FLOW
 C
 C MXCNPK1 : MAX. NO. OF DATA POINTS FOR CROSS-SECTIONAL GEOMETRY PROFILES
 C
 C PARAMETER (MXCNPK1=200)
 C
 C --- CONTROL INTEGERS FOR CHANNEL JUNCTIONS
 C
 C MXJTK1 : MAX. NO. OF CHANNEL JUNCTIONS
 C MXJTRK1 : MAX. NO. OF CHANNEL REACHES CONNECTED TO A JUNCTION
 C MXJTPK1 : MAX. NO. OF CHANNEL JUNCTION PROFILES
 C MXJTDK1 : MAX. NO. OF DATA POINTS ON THE PROFILES
 C MXNJTSK1 : MAX. NO. OF JUNCTION-RELATED OVERLAND BOUNDARY SIDES TO A JUNCTION
 C
 C PARAMETER (MXJTK1=500,MXJTRK1=50,MXJTPK1=50,MXJTDK1=100)
 C PARAMETER (MXNJTSK1=50)
 C
 C --- CONTROL INTEGERS FOR SUB-ELEMENT TRACKING FOR 1-D CHANNEL FLOW
 C
 C MXNPWK1 : MAX. NO. OF NODES FOR A SUB-ELEMENT TRACKING
 C
 C PARAMETER (MXNPWK1=11)
 C
 C --- CONTROL INTEGERS FOR HYDROGRAPH OF 1-D CHANNEL FLOW
 C
 C MXPNTK1 : MAX. NO. OF NODAL POINTS FOR THE LINE CROSS SECTION
 C MXLINK1 : MAX. NO. OF LINE CROSS SECTION CAN BE SELECTED
 C MXITPK1 : MAX. NO. OF DATA POINTS ON THE HYDROGRAPH
 C

C

C

cc

C

cc

C

C

cc

C

C

C

PARAMETER (MXSRPRK1=20,

PARAMETER (MYBPPBK1=20 MYBPPDPK1=20)

PARAMETER (MXAPPRK1=20,MXAPDPK1=20)

PARAMETER (MXDNPTK1=20)

CONTROL DETECTORS FOR C

cc

cc

cc

cc

C

C

C

C

C

C

PARAMETER (MXTNCK=MXNCHK*(MXNSIK*2+1),MXTNS

PARAMETER (MXTCSK=MXTNCK+MXNSITK+MXNSORK)

PARAMETER (MXAPPRK=20,MXAPDPK=20)

CONTROL INTEGERS FOR DESCRIBING FUNCTIONAL CURVES

MXXYSK : MAX NO OF CURES/SERIES

MAXYPR : MAX. NO. OF DATA POINTS FOR THE CURVES

PARAMETER (MAXYISK=300,MAXYPR=300)

C
D

C

c

C MXSBNP : MAX. NO. OF 3-D BOUNDARY NODES
 C MXSBES : MAX. NO. OF 3-D BOUNDARY ELEMENT SIDES
 C MXSTUBS : MAX. NO. OF 3-D TOTAL UNSPECIFIED BOUNDARY SIDES
 C MXSJBD : MAX. NO. OF GLOBAL NODES NEEDED TO DESCRIBE THE NODE-NODE CONNECTIVITY
 C MXSKBD : MAX. NO. OF GLOBAL ELEMENT NEEDED TO DESCRIBE NODE-ELEMENT CONNECTIVITY
 C MXSNTI : MAX. NO. OF TIME STEP SIZE
 C MXSDTC : MAX. NO. OF THE CHANGE OF TIME STEP SIZE
 C MXSMAT : MAX. NO. OF MATERIAL TYPE
 C MXSSPPM : MAX. NO. OF PARAMETERS NEEDED TO DESCRIBE PROPERTIES RELATED TO FLOW
 C COMPUTATION FOR ANY MATERIAL
 C MXSMPPM : MAX. NO. OF PARAMETERS NEEDED TO DESCRIBE PROPERTIES RELATED TO TRANSPORT
 C COMPUTATION FOR ANY MATERIAL
 C MXSRMP : MAX. NO. OF PARAMETERS NEEDED TO DESCRIBE PROPERTIES RELATED TO THE
 C IMPLEMENTATION OF RIVER BOUNDARY CONDITIONS IN FLOW COMPUTATION FOR ANY
 C RIVER BED MATERIAL
 C

PARAMETER(MXSNP=2079,MXSEL=2400,MXSBNP=882,MXSBES=880)

PARAMETER(MXSTUBS=4*MXSBNP)

PARAMETER(MXSJBD=27,MXSKBD=16,MXSNTI=10000,MXSDTC=20)

PARAMETER(MXSMAT=1,MXSSPPM=8,MXSMPPM=14)

PARAMETER(MXSRMP=8)

C
 C — CONTROL INTEGERS FOR 3-D FLOW SOURCE/SINK AND BOUNDARY CONDITIONS
 C

C MXSWNPF : MAX. NO. OF POINT SOURCES/SINKS
 C MXSWPRF : MAX. NO. OF PROFILES USED TO DESCRIBE POINT SOURCES/SINKS
 C MXSWDPF : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY POINT SOURCE/SINK PROFILE
 C MXSCNPF : MAX. NO. OF POINT CAUCHY BOUNDARY NODES
 C MXSCESF : MAX. NO. OF CAUCHY BOUNDARY SIDES
 C MXSCPRF : MAX. NO. OF PROFILES USED TO DESCRIBE CAUCHY BOUNDARY CONDITIONS
 C MXSCDPF : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY CAUCHY BOUNDARY PROFILE
 C MXSNNPF : MAX. NO. OF POINT NEUMANN BOUNDARY NODES
 C MXSNESF : MAX. NO. OF NEUMANN BOUNDARY SIDES
 C MXSNPRF : MAX. NO. OF PROFILES USED TO DESCRIBE NEUMANN BOUNDARY CONDITIONS
 C MXSNDPF : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY NEUMANN BOUNDARY PROFILE
 C MXSVNPF : MAX. NO. OF POINT VARIABLE BOUNDARY NODES
 C MXSVESF : MAX. NO. OF VARIABLE BOUNDARY SIDES
 C MXSVPRF : MAX. NO. OF PROFILES USED TO DESCRIBE VARIABLE BOUNDARY CONDITIONS
 C MXSDVPF : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY VARIABLE BOUNDARY PROFILE
 C MXSDNPF : MAX. NO. OF POINT DIRICHLET BOUNDARY NODES
 C MXSDPRF : MAX. NO. OF PROFILES USED TO DESCRIBE DIRICHLET BOUNDARY CONDITIONS
 C MXSDDPF : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY DIRICHLET BOUNDARY PROFILE
 C MXSRNPF : MAX. NO. OF POINT RIVER BOUNDARY NODES
 C MXSRPRF : MAX. NO. OF PROFILES USED TO DESCRIBE RIVER BOUNDARY CONDITIONS
 C MXSRDPF : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY RIVER BOUNDARY PROFILE
 C MXSRMAF : MAX. NO. OF BED MATERIALS ON THE RIVER BOUNDARY
 C MXSRESF : MAX. NO. OF RIVER BOUNDARY SIDES.
 C

PARAMETER(MXSWNPF=1,MXSWPRF=1,MXSWDPF=1)

PARAMETER(MXSCNPF=1,MXSCESF=1,MXSCPRF=1,MXSCDPF=1)

PARAMETER(MXSNNPF=1,MXSNESF=1,MXSNPRF=1,MXSNDPF=1)

PARAMETER(MXSVNPF=500,MXSVESF=300,MXSVPRF=5,MXSDVPF=6)

PARAMETER(MXSDNPF=300,MXSDPRF=4,MXSDDPF=6)

PARAMETER(MXSRNPF=1,MXSRPRF=1,MXSRDPF=1,MXSRMAF=1,MXSRESF=1)

C
 C — CONTROL INTEGERS FOR 3-D TRANSPORT SOURCE/SINK AND BOUNDARY CONDITIONS
 C

C MXSWNPT : MAX. NO. OF POINT SOURCES/SINKS
 C MXSWPRT : MAX. NO. OF PROFILES USED TO DESCRIBE POINT SOURCES/SINKS
 C MXSWDPT : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY POINT SOURCE/SINK PROFILE
 C MXSCNPT : MAX. NO. OF POINT CAUCHY BOUNDARY NODES
 C MXSCEST : MAX. NO. OF CAUCHY BOUNDARY SIDES
 C MXSCPRT : MAX. NO. OF PROFILES USED TO DESCRIBE CAUCHY BOUNDARY CONDITIONS
 C MXSCDPT : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY CAUCHY BOUNDARY PROFILE
 C MXSNNPT : MAX. NO. OF POINT NEUMANN BOUNDARY NODES

```

C MXSNEST : MAX. NO. OF NEUMANN BOUNDARY SIDES
C MXSNPRT : MAX. NO. OF PROFILES USED TO DESCRIBE NEUMANN BOUNDARY CONDITIONS
C MXSNDPT : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY NEUMANN BOUNDARY PROFILE
C MXSVNPT : MAX. NO. OF POINT VARIABLE BOUNDARY NODES
C MXSVEST : MAX. NO. OF VARIABLE BOUNDARY SIDES
C MXSVPRT : MAX. NO. OF PROFILES USED TO DESCRIBE VARIABLE BOUNDARY CONDITIONS
C MXSVDPT : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY VARIABLE BOUNDARY PROFILE
C MXSDNPT : MAX. NO. OF POINT DIRICHLET BOUNDARY NODES
C MXSDPRT : MAX. NO. OF PROFILES USED TO DESCRIBE DIRICHLET BOUNDARY CONDITIONS
C MXSDDPT : MAX. NO. OF DATA POINTS NEEDED TO DESCRIBE ANY DIRICHLET BOUNDARY PROFILE
C MXSNPW : MAX. NO. OF WORKING NODES USED FOR IMPLEMENTING THE 'IN-ELEMENT' PARTICLE
C TRACKING
C MXSELW : MAX. NO. OF WORKING ELEMENTS USED FOR IMPLEMENTING THE 'IN-ELEMENT' PARTICLE
C TRACKING
C
C PARAMETER(MXSWNPT=1,MXSWPRT=1,MXSWDPT=1)
C PARAMETER(MXSCNPT=1,MXSCEST=1,MXSCPRT=1,MXSCDPT=1)
C PARAMETER(MXSNNPT=1,MXSNEST=1,MXSNPRT=1,MXSNDPT=1)
C PARAMETER(MXSVNPT=500,MXSVEST=400,MXSVPRT=3,MXSVDPT=5)
C PARAMETER(MXSDNPT=300,MXSDPRT=3,MXSDDPT=5)
C PARAMETER(MXSNPW=125,MXSELW=64)
C
C ===== MAXIMUM DIMENSION BLOCK FOR GRAPHIC INTERFACE
C
C PARAMETER(MXPNTK=10,MXLINK=5,MXITPK=30)
C
C ===== MAXIMUM DIMENSION BLOCK FOR 1-D/2-D MAPPING
C
C MXN12NK : MAX. NO. OF OVERLAND NODES ASSOCIATED WITH A RIVER
C NODE.
C
C PARAMETER (MXN12NK=11)

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

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1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE July 1998		3. REPORT TYPE AND DATES COVERED Final report	
4. TITLE AND SUBTITLE A Numerical Model Simulating Water Flow and Contaminant and Sediment Transport in <u>W</u> ater <u>S</u> hed Systems of 1-D Stream-River Network, 2-D Overland Regime, and 3-D Subsurface Media (WASH123D: Version 1.0)				5. FUNDING NUMBERS	
6. AUTHOR(S) Gour-Tsyh (George) Yeh, Hwai-Ping (Pearce) Cheng, Jing-Ru (Ruth) Cheng, Hsin-Chi J. Lin, William D. Martin					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Civil and Environmental Engineering, The Pennsylvania State University, University Park, PA 16802; U.S. Army Engineer Waterways Experiment Station 3909 Halls Ferry Road, Vicksburg, MS 39180-6199				8. PERFORMING ORGANIZATION REPORT NUMBER Technical Report CHL-98-19	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Environmental Protection Agency Environmental Research Laboratory Athens, GA 30605				10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES Available from National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161.					
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.				12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) This report presents the development of a numerical model simulating water flow and contaminant and sediment transport in watershed systems of one-dimensional river/stream network, two-dimensional overland regime, and three-dimensional sub-surface media. The model is composed of two modules: flow and transport. Three options are provided in modeling the flow module in river/stream network and overland regime: the kinematic wave approach, diffusion wave approach, and dynamic wave approach. The kinematic and diffusion wave approaches are known to be numerically robust in terms of numerical convergency and stability; i.e., they can generate convergent and stable simulations over a wide range of ground surface slopes in the entire watershed. The question is the accuracy of these simulations. The kinematic wave approach usually produces accurate solutions only over the region of steep slopes. The diffusion wave approach normally gives accurate solutions over the region of mild to steep slopes. However, neither approach has the ability to yield accurate solutions over the region of small slopes, in which the inertial forces are no longer negligible compared to the gravitational forces. The kinematic wave approach cannot address the problems of backwater effects. On the other hand, a dynamic wave approach, having included all forces,					
(Continued)					
14. SUBJECT TERMS See reverse.				15. NUMBER OF PAGES 369	
				16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT		

13. (Concluded).

can theoretically have the potential to generate accurate simulations over all ranges of slopes in a watershed. The subsurface flow is described by Richard's equation where water flow through saturated-unsaturated porous media is accounted for .

In the transport module for the river/stream network and overland regime, both contaminant and sediment transport are taken into account. Dissolved chemicals are the only chemicals that may appear in both surface and subsurface systems. They may enter the subsurface system from the surface system through infiltration or from subsurface to surface through seepage. Chemical kinetics based on the collision theory is used to describe the interaction among chemicals.

Solving the diffusion wave flow equations employs the backward method of characteristics. All the nonlinear coefficient/source/sink terms are estimated along the flow characteristics. The Galerkin finite element method is used to discretize Richard's equation. The Picard method is applied to deal with the non-linearity of the flow equations. The predictor-corrector numerical scheme is employed to solve transport equations. The Newton-Raphson method is used to solve the set of algebraic equations describing chemical kinetics among all chemical species.

A total of fifteen groups of example problems were given in this report to demonstrate the capability of this model.

14. (Concluded)

Contaminant and sediment transport
Darcy's velocity
Diffusion wave
Galerkin finite element method
Newton-Raphson method
Overland flow
Picard method
Richard's equation
Subsurface flow
Watershed system